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Each dancing away, desiring,
Sea green oceans within to be lost,

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Or just remain a dream, an elusive dream...

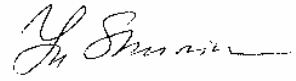
John's Scientific-Pantheist Poems

This 10th volume No.4 pays attention to solid state physics problems, which are really the topic of the day. Some particular tasks in computer modelling, applied mathematics and statistics are considered. Models of teaching technologies and distance education are also discussed.

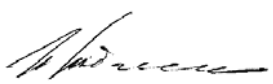
This means that our journal policy is directed on the fundamental and applied sciences researches, which is the basement of a full-scale modelling in practice.

We would like with this edition to emphasize 10 years of the existence of our Journal. We consider that our publishing activities are important for us. We hope also that the journal is interesting for research community, and we are open for collaboration.

EDITORS



Yu.N. Shunin



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Transport and Telecommunication Institute, Lomonosova 1, Riga, LV-1019, Latvia

THE ATOMIC AND ELECTRONIC STRUCTURE OF PURE AND DEFECTIVE $PbZrO_3$

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First principles DFT (Density Functional Theory) calculations have been performed using hybrid exchange-correlation functionals B3PW and B3LYP containing an admixture of non-local Fock exchange. Calculated equilibrium geometry of orthorhombic (antiferroelectric) PZ is in a good agreement with the recent experimental observations. The influence of point defects to the ferroelectric nature of PZ is modelled by incorporating of single F^0*-centre* (oxygen vacancy containing two electrons) into the bulk crystal. The computed electronic structures for both pure and defective PZ are discussed.

Keywords: *Density Functional Theory, F^0-centres*

1. Introduction

Lead zirconate is a typical antiferroelectric material which is proven to be very good candidate for applications involving actuation and high charge storage devices [1-6]. A field-induced ferroelectric phase transition in $PbZrO_3$ (PZ) is feasible due to a small free energy difference between the ferroelectric and the antiferroelectric phases [7, 8]. In order to shed some further light to the origin of the ferroelectric-antiferroelectric behavior of lead zirconate its crystal structure in the most common antiferroelectric phase has been calculated.

The antiferroelectric behaviour of lead zirconate has been discovered more than fifty years ago [9, 10], but up to now lead zirconate is one of the most studied materials. Lead zirconate has the Curie temperature of around 505 Kelvin. It is a promising material for future actuators and high energy capacitors. Lead zirconate is a mother compound of PZT solid solutions, which exhibit various piezo- and ferroelectric properties depending on concentration. Antiferroelectric-ferroelectric phase switching has been observed in lead zirconate thin films. Recently, lead zirconate thin films were suggested as promising candidates for application in a radiation environment, e.g. bolometer system for fusion devices [11].

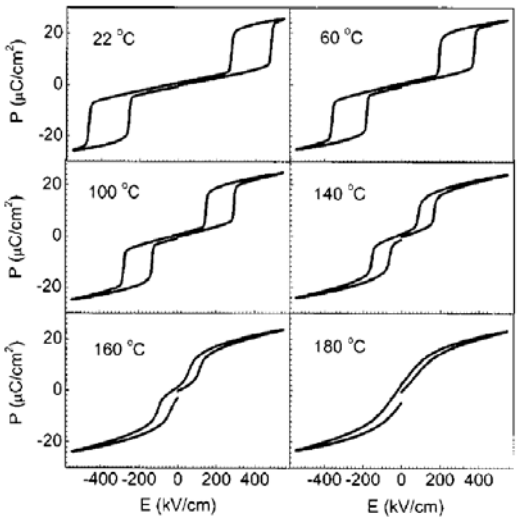

Figure 1. The temperature dependence of the polarization vs electric hysteresis loop of 900nm thick PbZrO3 thin films (measured at 1 kHz) (taken from Appl. Phys. Lett. 82 (2003) 2673)

The presence of defect substantially changes the atomic structure of material and thus, its electronic properties too. As it is shown in Figure 1 presence of surface, the two-dimensional defect with respect to perfect three-dimensional crystal obviously influences the antiferroelectric-ferroelectric phase switching. Figure 2 shows schematically the influence of point defect to orientation of polarization vector in ferroelectric domains.

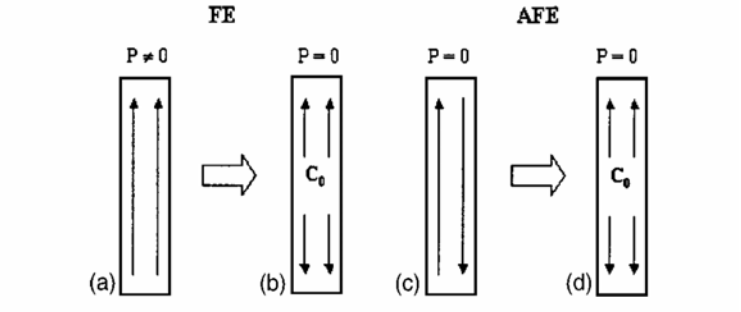

Figure 2. (a)–(c) Schematic view of the polarization vectors inside a polar region (domain) of a FE (a) and an AFE (c), (b) and (c) indicate the change of the polarization P caused by an oxygen vacancy C0 in the FE and in the AFE domain, respectively

The experimental studies on crystal structure of antiferroelectric lead zirconate agreed that orthorhombic (antiferroelectric) phase forms due to substantial antiparallel displacement of lead atoms along a-side of orthorhombic cell (Figure 3) and subsequent rotation of oxygen octahedra with respect to practically immovable zirconium atoms (Figure 4).

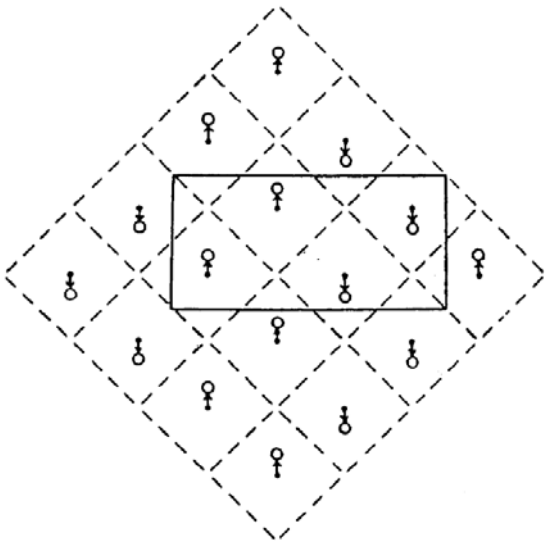

Figure 3. Crystal structure model of PbZrO3. Arrows represent the direction of shifts of Pb ions. The solid line shows an orthorhombic unit cell, and the dotted line shows pseudo cubic cells. (Taken from Ferroelectrics 266 (2002) 341)

The electronic properties for both cubic and orthorhombic PZ were calculated by Singh [13]. He used the local density approximation (LDA) and linearized augmented plane-wave (LAPW) method. Hybridization between O 2p and Zr 4d as well as O 2p and Pb 6s and 6p states in the cubic phase was determined. Singh obtained small energy difference (0.02 eV) between antiferroelectric and ferroelectric PZ structures. The cation positions were held rigid. Recently the structure of the antiferroelectric PZ was recalculated using LDA-LAPW approach but atomic coordinates were allowed to relax [15]. The results of later study are in good agreement with experiments [12]. Calculated energy difference between paraelectric cubic and antiferroelectric orthorhombic phases is 0.27 eV [15]. Leung and Wright have made the full-potential LDA-LAPW calculations to observe the influence of pressure in the phase transformation of PZ [15]. Their calculations also show the small energy difference between ferroelectric and antiferroelectric phases [14].

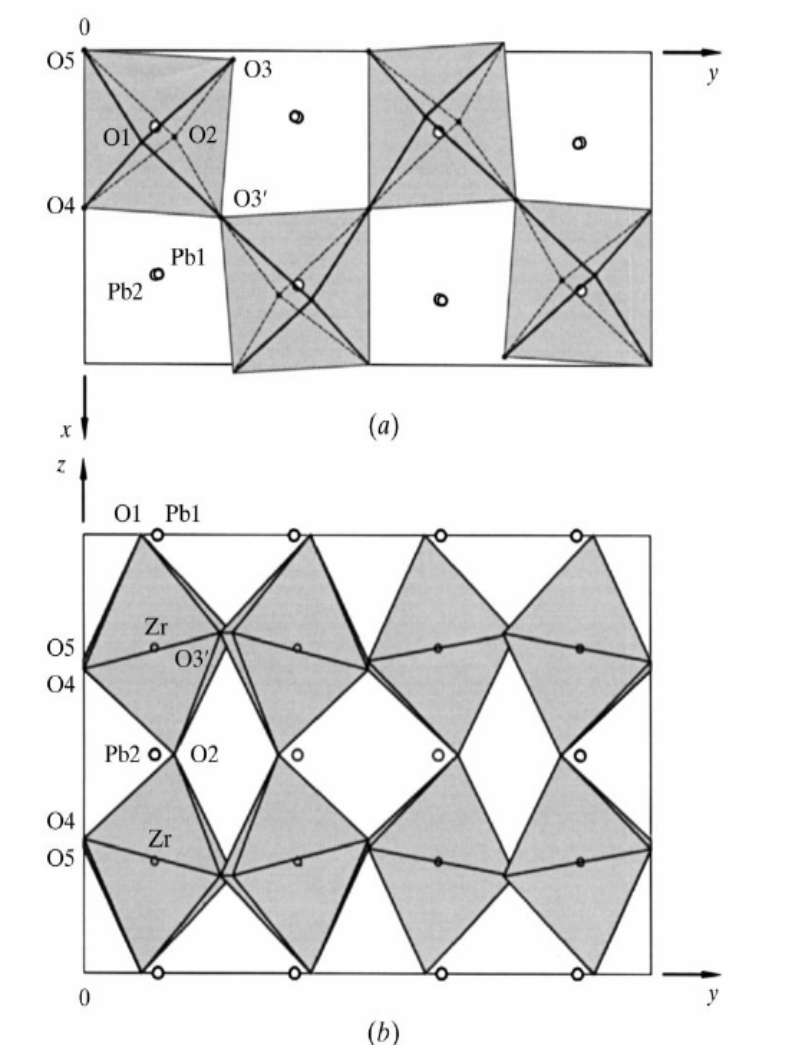

Figure 4. Projections of the superstructure of PbZrO3: (a) on 001 and (b) on 100. In (a) only the upper half of the unit cell is projected. (Taken from Acta Cryst. B54 (1998) 524)

In ABO_3 perovskites oxygen vacancies could be formed and their concentrations could be controlled by irradiation or thermal treatment. In PZ oxygen vacancies could be formed under neutron and ionizing irradiation [9]. Despite of their high importance, studies on point defects in lead zirconate are very scarce in the literature. As far as we know this is the first *ab initio* simulation on point defect in the bulk lead zirconate.

In this work we consider the atomic and electronic structure of bulk lead zirconate in its high-temperature cubic and low-temperature orthorhombic phase cubic PZ with F^o *centres* (neutral oxygen vacancies containing ~1.5 *e*). The electronic properties of perfect PZ crystal in both phases and cubic PZ with an isolated *F-centre* are compared.

2. Computational details

CRYSTAL-03 package is widely used now to perform comprehensive *ab initio* periodic calculations. Both HF and DFT methods implemented in these codes are realized via the self-consistent field (SCF) solution of the one-electron equations:

$$\hat{h}_i \varphi_{\mathbf{k}i}(\mathbf{r}) = \varepsilon_{\mathbf{k}i} \varphi_{\mathbf{k}i}(\mathbf{r}), \quad (1)$$

where crystalline orbitals of the *N*-electron system are expanded as linear combinations of a set of *m* Bloch functions built from local atom-centred Gaussian-type functions (GTFs):

$$\varphi_{\mathbf{k}i}(\mathbf{r}) = N\sum_{j=1}^{m} a_{ij}(\mathbf{k})\left(\sum_{\mathbf{g}} \chi_{\mathbf{g}j}(\mathbf{r})\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{g})\right), \quad (2)$$

where **k** is the wave vector of the irreducible representation of the group of crystal translations {**g**}. Atomic Gaussian-type functions $\chi_{\mathbf{g}j}(\mathbf{r})$ are defined as:

$$\chi_{\mathbf{g}j}(\mathbf{r}-\mathbf{A}_j) = \sum_{\mu}^{n_G} c_\mu G(\alpha_\mu; \mathbf{r}-\mathbf{A}_j-\mathbf{g}), \quad (3)$$

where $\mathbf{A}_j$ denotes the coordinate of nucleus in the zero cell of which atomic function $\chi_{\mathbf{g}j}(\mathbf{r})$ is centred; ***G***, c_μ and α_μ are normalized GTF, its coefficients and exponents, respectively which form the basis set.

The basis set for zirconium we took from CRYSTAL home page [16], while basis sets for lead and oxygen we took from our earlier study on lead titanate [20]. The inner core electrons of Pb and Zr atoms were described by Hay-Wadt effective core pseudopotentials taking into account the relativistic effect [19].

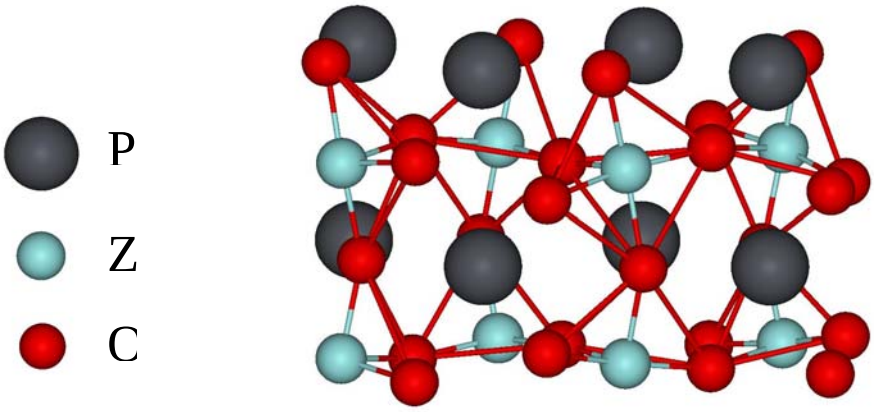

Figure 5. Modeled $PbZrO_3$ orthorombic *Pbam* structure

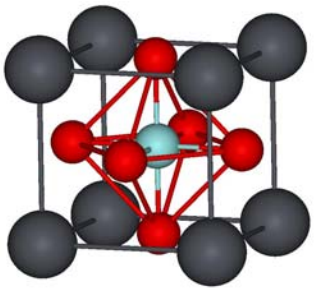

Figure 6. Unit cell of cubic (Pm3m) $PbZrO_3$

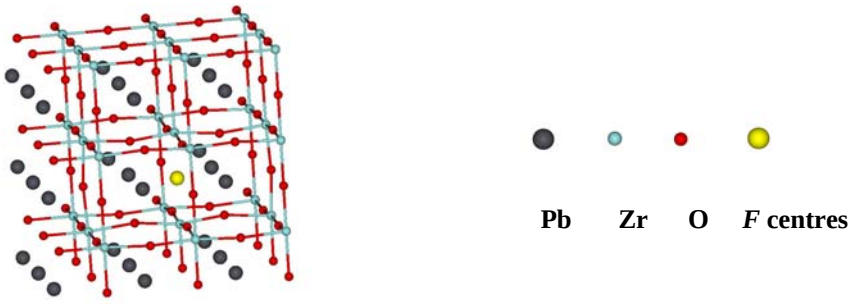

Figure 7. The cubic $PbZrO_3$ supercell with F^0-centre defect as it was modelled

In Figure 5 an orthorhombic unit cell is shown exactly as we calculated it. At high temperatures, above around 520 Kelvin, lead zirconate possesses high symmetry simple cubic phase (Figure 6). To simulate an isolated *F-centre* in lead zirconate we extend the simple cubic cell to 3x3x3 supercell in order to construct large enough supercell containing 135 atoms (Figure 7).

To model the *F-centre* defect a "ghost" basis set was used [16]. This means that O atom is removed but its basis set is left. The ghost basis set allows more physical redistribution of electron density inside and in the vicinity of the vacancy. The equilibrium geometry was received implemented in the *CRYSTAL* code analytical optimization method. CRYSTAL ParOptimize code was used to optimize lattice constants [20]. This code implements conjugated gradient optimization with numerical computation of derivatives [21]. The reciprocal space integration was performed by a sampling the Brillouin zone with the 8x8x8 Pack-Monkhorst and Gilat meshes for a cubic unit cell [22, 23], 6x6x6 for an orthorhombic unit cell, and 4x4x4 for 135-atom cubic SC with a defect. Such a sampling provides the balanced summation in direct and reciprocal lattices.

CRYSTAL allows us to perform *ab initio* calculations using both Hartree-Fock (HF) and (DFT) methods implementing the self-consistent field (SCF) solution of the corresponding one-electron equation [16]. To achieve scalable results it is important to choose appropriate exchange-correlation functional for Crystal calculations implementing DFT method. In our calculation we employed DFT method accompanied with hybrid exchange-correlation functional containing an admixture of exact non-local Fock exchange:

CRYSTAL code realizes partial incorporation of the exact non-local HF exchange into the non-local DFT exchange functional, with varying mixing ratio. We have used both B3PW (eq. 4) and B3LYP (eq. 6) exchange-correlation energy functional:

$$E_{xc} = (1-a_h)E_x^{LDA} + a_x E_x^{Becke} + a_h E_x^{HF} + a_c E_c^{PWGGA}, \quad (4)$$

$$E_{xc} = (1-a_h)(E_x^{LDA} + a_x E_x^{Becke}) + a_h E_x^{HF} + (1-a_c)E_c^{VWN} + a_c E_c^{LYP}, \quad (5)$$

where a_h is input parameter of the HF/DFT exchange mixing; a_x and a_c are input parameters of the DFT exchange (x) and correlation (c) non-locality (GGA/LDA), respectively; PWGGA and LYP mean non-local correlation functional of the Perdew-Wang and Lee-Yang-Parr.

3. Results and discussion

Table 1 compares our calculated atomic coordinates of orthorhombic lead zirconate crystal with those experimentally observed (right column) [12, 13]. Coordinates calculated by means of both B3PW and B3LYP are in good agreement with experiment, the disagreement mainly is less than one hundredth of fractional unit, while lattice constant are better reproduced by B3PW. Thus, it gives us a ground to choose B3PW for further calculations of electronic properties.

TABLE 1. Experimental data are taken from Fujishita et al., J. Phys. Soc. Jpn. 72 (2003) 1426 [14]. Energy gain due to *Pm3m* – Pbam phase transition is 0.39 eV per formula unit

	B3PW			B3LYP			Experimental, 10 K		
Atom	x	y	z	x	y	z	x	y	z
Pb1	0.6909	0.1234	0.0000	0.6926	0.1223	0.0000	0.6991	0.1228	0.000
Pb2	0.7063	0.1274	0.5000	0.7068	0.1278	0.5000	0.7056	0.1294	0.5000
Zr	0.2406	0.1246	0.2500	0.2410	.01248	0.2500	0.2414	0.1248	0.2486
O1	0.2797	0.1579	0.0000	0.2799	0.1592	0.0000	0.2756	0.1560	0.0000
O1'	0.3103	0.0934	0.5000	0.3111	0.0924	0.5000	0.3011	0.0956	0.5000
O2	0.0393	0.2646	0.2816	0.0395	0.2646	0.2838	0.0317	0.2622	0.2798
O3	0.0000	0.5000	0.1972	0.0000	0.5000	0.1949	0.0000	0.5000	0.2026
O4	0.0000	0.0000	0.2343	0.0000	0.0000	0.2324	0.0000	0.0000	0.2293
Orthorhombic PZ lattice constants									
a, Å	5.9411			5.9868			5.8736		
b, Å	11.8024			11.8630			11.7770		
c, Å	8.2561			8.3243			8.1909		
Cubic PZ lattice constants									
a_0, Å	4.177			4.209			4.1614		

The Mulliken atomic charges differ from formal ionic charges mainly because of two reasons: Firstly, because the Mulliken scheme is sensitive to outer diffuse exponents in Gaussian basis set, and secondly, due to partly covalent nature of bonds between oxygen and cations. The covalence of lead-oxygen bond is widely discussed in the literature. The positive bond population of lead-oxygen bond in cubic lead zirconate indirectly confirms that statement. However, covalence of lead-oxygen bond is weaker than covalence of oxygen-zirconium bond. Repulsion between neighbour oxygens in ABO_3 perovskites is expected. We would like to stress that population of lead-oxygen bond in lead zirconate more than two times larger than in lead titanate as it follows from our calculations [20]. In Table 3 it is shown that covalence in lead-oxygen and zirconium-oxygen bonds increases as orthorhombic phase transition occurs, and thus, can play important role in formation of antiferroelectricity in lead zirconate.

TABLE 2

Atomic charges		
Atom	(x,y,z)	q,e
Pb	(0,0,0)	1.30
Zr	(0.5,0.5,0.5)	2.07
O	(0,0.5,0.5)	-1.12
Bond populations		
Bond	p, me	
O-Pb	36	
O-Zr	100	
O-O	-20	

TABLE 3

Atomic charges								
Atom	(x,y,z)	q,e	Atom	(x,y,z)	q,e	Atom	(x,y,z)	q,e
Pb1	(0.69,0.12,0)	1.30	O1	(0.28,0.16,0)	-1.16	O3	(0,0.5,0.2)	-1.21
Pb2	(0.71,0.13,0.5)	1.29	O1’	(0.31,0.09,0.5)	-1.18	O4	(0,0,0.23)	-1.09
Zr	(0.24,0.12,0.25)	2.18	O2	(0.04,0.26,0.28)	-1.15			
Bond population								
Bond	p, me		Bond	p, me		Bond	p, me	
Pb1-O1	76		Ze-O4	198		O4-O3	-20	
Pb2-O1’	76		O1-O3	-96				
Zr-O2	162		O1’-O2	-84				

Both Tables show the calculated Mulliken atomic charges and bond populations for paraelectric () and ferroelectric phases () of lead zirconate

In the calculated differential charge density maps (Figures 8a, 9a, 8b, 9b) red lines are responsible for covalence. The rich red regions between oxygens and zirconiums for both cubic and orthorhombic lead zirconate are shown, while between lead and oxygen the black isodensity curve is shown, indicating the zero-charged border. It means that only weak covalence can be expected in the lead-oxygen bond.

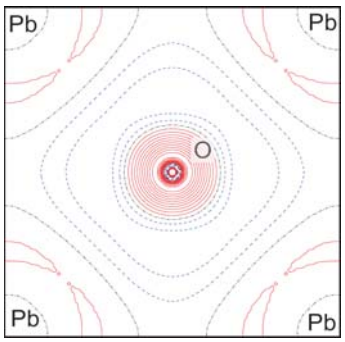

Figure 8.a

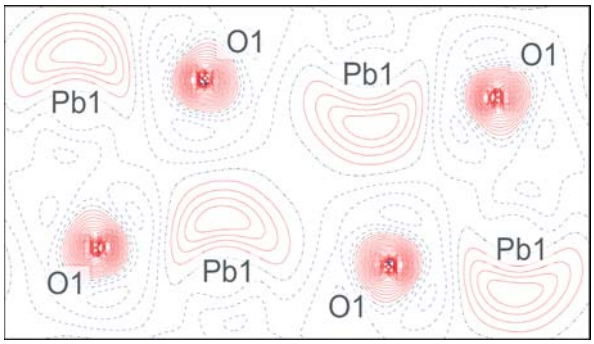

Figure 9.a

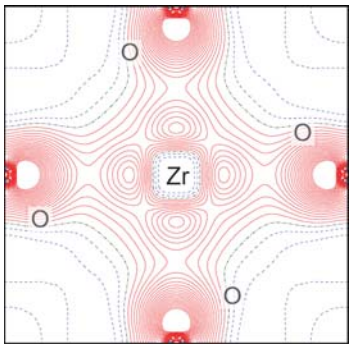

Figure 8.b

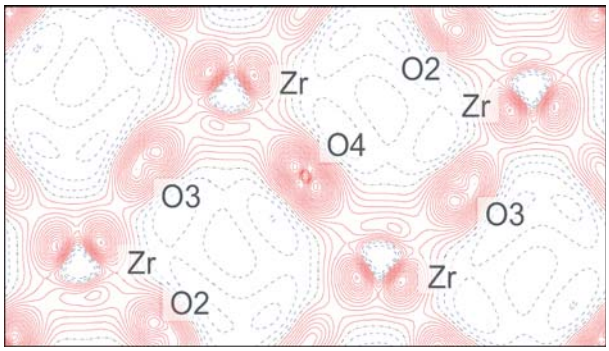

Figure 9.b

Figures 8.a and 8.b show difference in electronic charge density maps for the cubic PZ and Figures 9.a and 9.b for orthorhombic PZ

In Figure 10 there are the densities of states (DOS) calculated for both cubic and orthorhombic phases of lead zirconate. In both cases the valence band consist mainly of oxygen 2p states with small contribution of zirconium 4d and lead 5p states. The peak of zirconium 4d states around -4.5 eV denotes the hybridization of zirconium 4d and oxygen 2p states which are responsible for covalence effect in zirconium-oxygen bond, while the small presence of lead states confirms the weak covalence of lead-oxygen bond. For orthorhombic structure the region at the minus one eV mainly consist of oxygen 2p and lead 6s orbitals. The regions just below the valence band mainly consist of lead 5s orbitals. The bottom of conduction band consists of lead 6p, zirconium 4d, and a little bit of oxygen 2p orbitals.

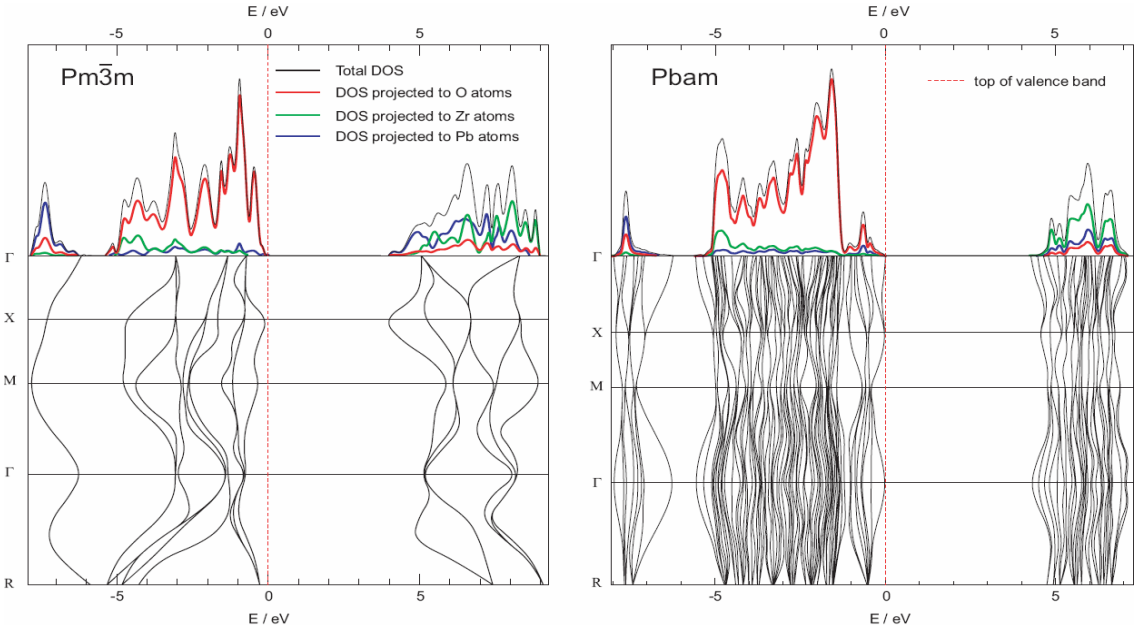

Figure 10. The densities of states and band structures calculated for both cubic and orthorhombic phases of lead zirconate

In defective PZ structure 8 nearest to *F-centre* atomic spheres were freely relaxed along symmetry-allowed directions. The displacements are summarized in Table 4. Here we would like to stress that zirconium atoms which practically do not move, while nearest lead atoms exhibit colossal shift of 0.18 Å toward *F-centre* and thus give rise to subsequent rotation of oxygen octahedron. It is commonly accepted that antiparallel displacement of lead atoms in orthorhombic lead zirconate structure is responsible for its antiferroelectric behaviour; therefore such a shift of leads induced by a vacancy should influence the ferroelectricity in defective lead zirconate.

TABLE 4. The displacement of atoms in the cubic PbZrO3 supercell with F^0*-centre* defect

		Displacement, Å		
Sphere	R, Å	x	y	z
1 (2Zr)	2.11	0.00	0.00	0.02
2 (4Pb)	2.70	-0.18	-0.18	0.00
3 (8O)	2.79	0.00	-0.03	-0.21
4 (2O)	4.14	0.00	0.00	-0.04
5 (4O)	4.32	0.00	0.14	0.00
6 (8Zr)	4.69	0.00	0.03	0.00
7 (8Pb)	5.12	0.00	0.00	0.00
8 (16O)	5.16	-0.01	-0.01	0.12

In Table 5 the Mulliken charges of atoms nearest to *F-centre* are shown. We would like to stress that the oxygen vacancy attracts ~0.7e, and the remaining electron density from the missing O^{2-} is localized mostly on 4 nearest Pb atoms. The charge density map (Figure11) confirms our conclusion. The blue curves go through the centres of lead atoms, as well as through the nearest zirconiums, which attract some density to themselves.

TABLE 5. Mulliken charges of atoms nearest to *F-centre*

Atomic charges		
Sphere	R, Å	q, e
0, F^0	0.00	-0.68
1 (2Zr)	2.11	2.09
2 (4Pb)	2.70	1.17
3 (8O)	2.79	-1.14
4 (2O)	4.14	-1.12
5 (4O)	4.32	-1.12
6 (8Zr)	4.69	2.08
7 (8Pb)	5.21	1.29
8(16O)	5.16	-1.12
Bond population		
Bond		p, me
F^0-Zr(1)		-18
F^0-Pb(2)		168
F^0-O(3)		-16
Pb(2)-O(3)		18
Pb(2)-O(53)		34

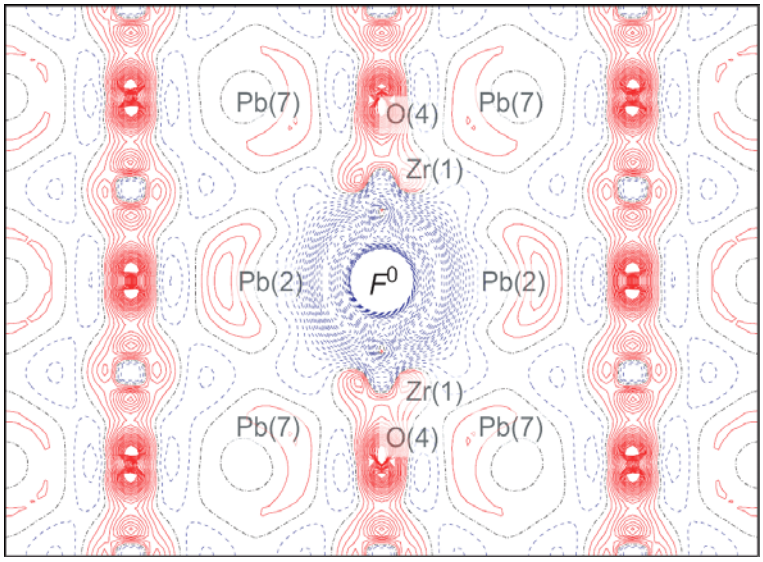

Figure 11. The density of states of lead zirconate containing *F-centre*

The density of states of lead zirconate containing *F-centre* (Figure 12) is very similar to the DOS of cubic lead zirconate. The defect level is placed in the middle of a band gap. Defect level consists of lead 6s and 6p orbitals as well as of small admixture of zirconium 4d electrons. This additionally confirms our conclusion drawn from Mulliken analysis.

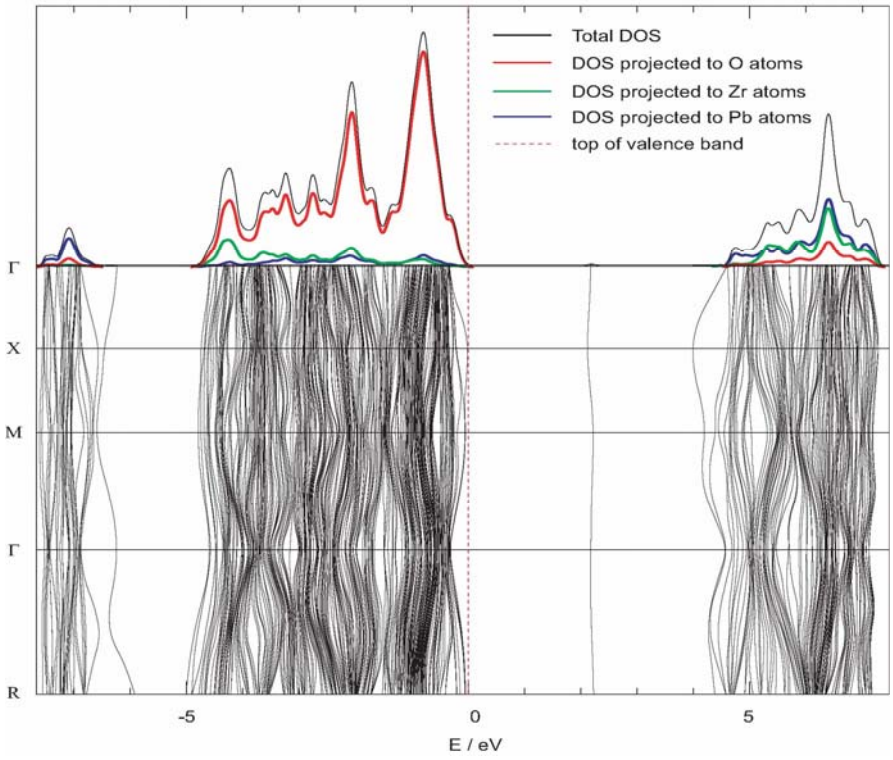

Figure 12. The densities of states and band structure calculated for both cubic and orthorhombic phases of lead zirconate

The defect level is practically flat; there is a small dispersion (0.14 eV) over the Brillouin zone. This means, that the interaction between the periodic *F-centres* in the model of 135-atom SC can be neglected for the qualitative description of isolated defect in PZ.

Conclusion

In this study we used B3PW and B3LYP exchange-correlation functional within DFT formalism as implemented in the CRYSTAL code. The atomic and electronic structures of pure lead zirconate in its high-temperature cubic and low-temperature orthorhombic and cubic lead zirconate structure containing a single *F-centre* were calculated. Calculated atomic coordinates and lattice parameters for perfect lead zirconate are in good agreement with those experimentally observed. The Pb-O covalence was estimated using the electronic charge redistribution for bulk lead zirconate. The covalence increases with the transition toward the orthorhombic phase. Formation of a *F-centre* defect in cubic lead zirconate causes a substantial shift of 0.25 Å of the nearest lead atoms towards the vacancy. 0.68e is localized in the oxygen vacancy. Defect level is located in the middle of the band gap. The presence of the point defects affects atomic polarization in lead zirconate and influences its ferroelectric properties.

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References

[1] Sengupta S. S., Roberts D., Li J., Kim M. C., Payne D. A. (1995) Field-induced phase switching and electrically driven strains in sol-gel derived antiferroelectric (Pb,Nb)(Zr,Sn,Ti)O_3 thin layers. *J. Appl. Phys.* **78** (2), 117-1177.

[2] Yamakawa K., Trolier-McKinstry S., Dougherty J. P., Krupanidhi S. B. (1995) Reactive magnetron co-sputtered antiferroelectric lead zirconate thin films. *Appl. Phys. Lett.* **67** (14), 1014-2016.

[3] Jang J. H, Yoon K. H., Shin H. J. (1998) Electric fatigue in solgel prepared Pb(Zr,Sn,Ti)NbO_3 thin films. *Appl. Phys. Lett.* **73** (13), 1823-1825.

[4] Xu B., Moses P., Pai N.G., Cross L.E. (1998) Charge release of lanthanum-doped lead zirconate titanate stannate antiferroelectric thin films. *Appl. Phys. Lett.* **72** (5), 593-595.

[5] Xu B., Ye Y., Cross L. E. (2000) Dielectric properties and field-induced phase switching of lead zirconate titanate stannate antiferroelectric thick films on silicon substrates. *J. Appl. Phys.* **87** (5), 2507-2515.

[6] Seveno R., Gundel H. W., Seifert S. (2001) Preparation of antiferroelectric $PbZr_xTi_{1-x}O_3$ thin films on LaSrMnO3-coated steel substrates. *Appl. Phys. Lett*. **79** (25), 4204-4206.

[7] Bharadwaja S. S. N., Krupanidhi S. B. (2001) Backward switching phenomenon from field forced ferroelectric to antiferroelectric phases in antiferroelectric $PbZrO_3$ thin films. *J. Appl. Phys.* **89** (8), 4541-4547.

[8] Zhai J., Chen H. (2003) Direct current field and temperature dependent behaviors of antiferroelectric to ferroelectric swithcing in highly (100)-oriented $PbZrO_3$ thin films. *Appl. Phys. Lett.* **82** (16), 2673-2675.

[9] Sawaguchi E. (2002) Lead zirconate – half a century ago. *Ferroelectrics* **266**, 341-353.

[10] Fujishita H. (2002) Order parameters in the structural phase transition of antiferroelectric PbZrO3. *Ferroelectrics* **266,** 27-40.

[11] Bittner R., Humer K., Weber H. W., Kundzins K., Sternberg A., Lesnyh D. A., Kulikov D. V., Trushin Y. V. (2004) Oxygen vacancy defects in antiferroelectric $PbZrO_3$ thin film heterostructures after neutron irradiation. *J. Appl. Phys.* **96**, 3239-3246.

[12] Singh D.J. (1995) Structure and energetics of antiferroelectric $PbZrO_3$. *Phys. Rev. B* **52** (17) 12559-12563.

[13] Johannes M. D., Singh D. J. (2005) Crystal structure and electric field gradients of PbZrO3 from density functional calculations. *Phys. Rev. B* **71,** 212101–1–21210–4.

[14] Fujishita H., Ishikawa Y., Tanaka S., Ogawaguchi A., Katano S. (2003) Crystal structure and order parameters in the phase transition of antiferroelectric PbZrO3. *J. Phys. Soc. Jpn.* 72 (6), 1426-1435.

[15] Leung K., Wright A F. (2002) Lead zirconate at ambient and high pressure. *Ferroelectrics* **281,** 171-186.

[16] Saunders V. R., Dovesi R., Roetti C., Orlando R., Zicovich-Wilson C. M., Harrison N. M., Doll K., Civalleri B., Bush I. J., D'Arco Ph., Llunell M. (2003) CRYSTAL 2003: User's Manual. Universita di Torino, Torino – http://www.crystal.unito.it/ (Aug. 2003).

[17] Piskunov S., Heifets E., Eglitis R. I., Borstel G. (2004) Bulk properties and electronic structure of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$ perovskites: An *ab initio* HF/DFT study. *Comp. Mat. Sci.* **29** (2), 165-178.

[18] Hay P. J., Wadt W. R. (1984) *Ab initio* effective core potentials for molecular calculations. Potentials for the transition metal atoms Sc to Hg. *J. Chem. Phys*. **82** (1), 270-283.

[19] Hay P. J., Wadt W. R. (1984) *Ab initio* effective core potentials for molecular calculations. Potentials for main group elements Na to Bi. *J. Chem. Phys.* **82** (1), 284-298.

[20] Heifets E., Eglitis R. I., Kotomin E. A., Maier J., Borstel G. (2001) *Ab initio* modeling of surface structure for $SrTiO_3$ perovskite crystals. *Phys. Rev. B* **64**, 23541-23547.

[21] Press W. H., Teukolsky S. A., Vetterling W. T., Flannery B. P. (1997) *Numerical Recipes in Fortran77*. 2nd edition. Cambridge, MA.: Cambridge Univ. Press.

[22] Monkhorst H. J., Pack J. D. (1976) Special points for Brillouin-zone integrations. *Phys. Rev. B* **13** (12), 5188-5192.

[23] Gilat G. (1982) General analytic method of zone integration for joint densities of states in metals, *Phys. Rev. B* **26** (4), 2243-2246.

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PROBLEM OF CLUSTER EMBEDDING IN CRYSTALLINE LATTICE

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General problem "subsystem in the field of the frozen remaining part of the whole electron system" is investigated in the framework of one-electron approximation. Orthogonality restrictions are not imposed on one-electron wave functions. Consideration is general for every task of this type (cluster and the rest of crystal, fragment of a molecule and the remaining part of it, valence and core electrons, etc.).

Total energy of the whole system (cluster + the rest of system) is expressed in terms of non-orthogonal one-electron wave functions. Equations for the cluster wave functions are obtained directly from variation of the total energy expression subject to the condition that wave functions of the rest of system are known and fixed. Mutual orthogonality constraints are not imposed during variation. Homogeneous equations resulting directly from general procedure are obtained first. Then they are transformed to the eigenvalue problem equations. Particular case of these equations giving mutually orthogonal one-electron wave functions of the cluster staying to be non-orthogonal to those of the remaining system is found. The remaining system wave functions are found not to be solutions of these equations.

Vacant solutions of the equations are studied. Initial equations are shown to have different structure for vacant and occupied cluster states. Initial equations are further modified in the way leading to the same structure for both occupied and vacant states and keeping occupied states unchanged.

Keywords: *Quantum-chemical simulation, embedded molecular cluster model, non-orthogonal one-electron wave functions, localised molecular orbitals, theory of pseudopotentials*

1. Introduction

When we treat infinite or very large electron systems we have to develop approaches giving us opportunity to transform our task to that for small finite part of the whole electron system. Considering main problems we have to deal with when our system has no translation symmetry, so we cannot use it to simplify the task.

Point defect in a crystal is an example of such system. The description of a crystal with a point defect is based on an intuitive assumption that the presence of the defect in the crystal alters significantly only a finite region of the crystal, including the defect and several spheres of its nearest surrounding. The whole system, i.e. the electrons and nuclei of the crystal with a point defect, may be split on two subsystems: the electrons and nuclei of the defect and its vicinity, and the electrons and nuclei of the remaining crystal. The first subsystem is finite and may be considered as a cluster in the field of the remaining crystal. Electronic and spatial structures of the cluster are calculated using quantum-chemical methods. The second subsystem (remaining crystal) is infinite, and its description is impossible without further approximations and assumptions.

Biological molecule (like DNA or protein) is another example of such system. To solve task for the whole system we also have to split the system on two parts: small fragment of the molecule and the remaining part of it. To treat large remaining part of the molecule we have to make further approximations. While small fragment of the molecule may be considered as a cluster in the field of the rest of system.

There are two different approaches permitting one to treat the task "cluster in the field of the remaining system". One of them is based on the Green functions technique. Hartree-Fock equations for one-electron wave functions of the crystal with point defect are transformed to those for the Green function of the whole system (cluster + remaining part of crystal). Then the task for the infinite system is converted to the task for its finite part (the cluster with the point defect). Short-range character of the crystal perturbation created by the defect is used substantially to carry out the conversion. This kind of approach is employed, for example, by C. Pisani with co-workers in EMBED code [1-3]. It works well for metals, semiconductors and insulators with covalent type of chemical bonding, where there are no charged defects. In the case of ionic and ion-covalent systems, where defects usually possess electric

charge or dipole moment, long-range character of the perturbation created by the defects is substantial. At present moment there are no clear ideas of how to treat the case with long-range perturbation applying Green functions technique. Problems of this type (how to describe response of the rest of system) will exist for every system treated by Green functions technique.

But there is an alternative approach that makes it possible to take into account long-range perturbation of the crystal by the defect located in the cluster region, treating it as polarisation of the remaining part of the crystal. This approach is so-called embedded molecular cluster (EMC) model, main ideas of which are described by L.N. Kantorovich [4]. It is based on the concept of localised electron groups and structural elements (SE). The cluster is considered as an entire system, but the remaining part of crystal is split on SE. Realisation of the EMC model assumes quite good localisation of the cluster wave function in the cluster region, while the remaining crystal wave function should be localised in the region of the remaining part of crystal. It requires that the crystal be composed of well-defined SE with well-localised wave functions. Central idea is that the wave function of the whole system (cluster + remaining part of crystal) is an antisymmetrised product of the cluster wave function and that of the remaining part of crystal. It allows us to divide the task for the whole system on two tasks:
(1) "cluster in the field of the remaining part of crystal" (embedding)
and
(2) "the remaining part of crystal under the influence of cluster with the defect" (response).

Trying to solve the first of these tasks and to obtain equations for the cluster one-electron wave functions, we face with general problem of description of "subsystem in the field of the remaining part of the whole electron system". Task for the cluster and the remaining part of crystal is a particular case of problem of this kind. Other possible cases may be, for example, fragment of a polymer and the remaining part of it, valence and core electrons, etc. All these systems have similar features and may be treated in the framework of general concepts of EMC model. Cluster, fragment of a polymer, valence electrons may be treated as entire quantum-chemical system. It may be considered to build the remaining part of a whole system (the rest of crystal, the remaining part of polymer, core electrons) of SE (SE of perfect crystal, building blocks (fragments) of polymer, and core electrons of separate atoms). So, general approach of EMC model permits us to obtain embedding equations for all the tasks of this kind.

At present, approaches employing the strong orthogonality constraints have been developed [4-10]. However, non-orthogonal wave functions of SE may turn out to be more localised than orthogonal ones. (See, for example, work of Anderson [11].) It is significant for practical applications, because expansion of a more localised wave function requires a smaller basis set.

Adams and Gilbert have investigated the case of non-orthogonal one-electron wave functions with arbitrary degree of localisation [12-16]. Adams and Gilbert have treated self-consistent solutions for the whole system and then searched for a particular form of general equations leading to the separation of the whole system on SE. Our consideration of this problem differs from the approaches based on Adams-Gilbert equations. Unlike Adams-Gilbert theory, we do not imply that the wave functions of the rest of system are self-consistent solutions of the equations for the whole system (cluster + the rest of system). Our approach permits us to use approximations for the rest of system, keeping equations for the cluster mathematically correct. It is significant for practical applications because when we describe the rest of system we are pressed to make approximations.

Using direct variational approach in our earlier works [17, 18] we obtained embedding equations for the cluster one-electron wave functions. The total energy of the whole system (cluster + remaining part of system) was expressed in terms of non-orthogonal one-electron wave functions. Equations for the cluster wave functions were obtained directly from variation of the total energy expression subject to the condition that wave functions of the remaining part of system are known and fixed. Mutual orthogonality restrictions were not imposed during variation. Then homogeneous equations resulting from variation procedure were transformed to eigenvalue problem equations. Particular case of these equations describing mutually orthogonal one-electron wave functions of the cluster staying to be non-orthogonal to those of the rest of system was found. Using these embedding equations we have developed modified embedding scheme and have demonstrated that consistent use of this scheme may radically reduce boundary effects in EMC model [18].

Further applications of EMC model require us to go beyond one-electron approximation and to use one of existing methods including many-electron correlation effects into consideration (to calculate optical transition energies or magnetic resonance effects, for example). To apply any of these methods, we need initial eigenvalue equations giving the same structure and the same degree of localisation for both vacant and occupied cluster states. In the present work we study occupied and vacant solutions of the cluster embedding equations proposed by us earlier [17, 18]. Our final goal is equations giving us both occupied and vacant cluster states of the same structure and the same degree of localisation.

2. Cluster embedding equations

Start with review of the most significant results of our earlier works [17, 18] without detailed proof and complete our study with recent new results.

2.1. GENERAL EQUATIONS

Consider a system of N electrons within the one-electron approximation. Assume that many-electron wave function of the system is represented by a single Slater determinant (this corresponds to calculation of an open shell system by unrestricted Hartree-Fock method). A one-determinant wave function is known to be invariant with respect to arbitrary non-singular linear transformation of the one-electron wave functions (spin-orbitals) the determinant is composed of [19, 20]. The existence of such transformation allows us to describe a many-electron system by localised one-electron wave functions instead of delocalised ones keeping the many-electron wave function unchanged. A particular case of the transformation is transformation of Bloch wave functions to Wannier wave functions for perfect crystals, when the transformation matrix is unitary, and wave functions remain orthogonal. In the present work, we consider the most general case when the transformation matrix leading to localised wave functions is not unitary and the localised wave functions are not orthogonal.

Assume, next, that the transformation of one-electron wave functions to localised ones has been carried out, and divide our electron system on two subsystems (cluster and the remaining system) in the same manner as it is usually done in the EMC model [4]. Then the spin-orbitals of the whole electron system $\left|\Psi_i\right\rangle$, $i\in$c+r, are split on two groups: $\left|\psi_i\right\rangle$, $i\in$c: localised in the cluster region, and $\left|\varphi_i\right\rangle$, $i\in$r: localised in the region of the remaining part of system. Main assumption of the EMC model, namely, that the wave function of the whole electron system is an anti-symmetries product of the cluster wave function and the remaining system wave function, within one-electron approximation is valid automatically without any additional assumptions. The total energy of the many-electron system within one-electron approximation with non-orthogonal one-electron wave functions is written in the following way:

$$E = \int h(1)\rho(1|2)\big|_{2=1} d1 + \tfrac{1}{2}\int g(1,2)[\rho(1|1)\rho(2|2) - \rho(1|2)\rho(2|1)]d1d2\,, \qquad (1)$$

where $\rho(1|2) = \sum_{i,j\in c+r} \Psi_i(1)\left(S^{-1}\right)_{ij}\Psi_j^*(2)$ is the one-electron density;

$h(1) = T(1) + V(1)$ includes the electron kinetic energy operator $T(1)$ and the operator $V(1)$ which describes the interaction of the electrons and nuclei;

$g(1,2) = \left|\vec{r}_1 - \vec{r}_2\right|^{-1}$ is the operator for interaction between electrons;

and $S_{ij} = \left\langle \Psi_i \middle| \Psi_j \right\rangle = \int \Psi_i^*(1)\Psi_j(1)d1$ are the one-electron wave functions overlap matrix elements. Electron coordinates includes both spatial and spin variables, the integration is carried out over both of them.

Requiring that the total energy variation δE is zero for arbitrary variations of the cluster wave functions $\delta\psi_l$ and $\delta\psi_k^*$ we come to the following system of equations:

$$\sum_{l\in c+r}(1-\rho)F\left|\Psi_l\right\rangle\left(S^{-1}\right)_{lk} = 0\,,\ k\in\text{c}, \qquad (2)$$

where

$$\rho = \sum_{i,j\in c+r}\left|\Psi_i\right\rangle\left(S^{-1}\right)_{ij}\left\langle\Psi_j\right| \qquad (3)$$

is one-electron density operator,
F is Fock operator,

$$F\left|\psi(1)\right\rangle = h(1)\left|\psi(1)\right\rangle + \int \rho(2|2)g(1,2)\left|\psi(1)\right\rangle d2 - \int \rho(1|2)g(1,2)\left|\psi(2)\right\rangle d2\,.$$

Eqs. (2) are usual equations resulting from partial variation of the total energy [21, 22]. We transform them further to get in the left side operator acting on the cluster wave functions. After multiplying each equation by $S_{ki} = \langle \psi_k | \psi_i \rangle$ and summing over *k* we obtain the equivalent system of equations:

$$\sum_{k\in c} \sum_{l\in c+r} (1-\rho) F |\Psi_l\rangle \left(S^{-1}\right)_{lk} \langle \psi_k | \psi_i \rangle = 0, \quad i \in \text{c}.$$

Define the following operators:

$$P_c = \sum_{i\in c} \sum_{j\in c+r} |\psi_i\rangle \left(S^{-1}\right)_{ij} \langle \Psi_j | \tag{4}$$

and

$$P_r = \sum_{i\in r} \sum_{j\in c+r} |\varphi_i\rangle \left(S^{-1}\right)_{ij} \langle \Psi_j | . \tag{5}$$

It is easy to see that $P_c + P_r = \rho = P_c^+ + P_r^+$. Then our system of equation may be rewritten as

$$(1-\rho) F P_c^+ |\psi_i\rangle = 0, \ i \in \text{c}, \qquad \text{(nonhermitean form)} \tag{6}$$

or

$$\left([1-P_r] F [1-P_r]^+ - P_c F P_c^+ \right) |\psi_i\rangle = 0, \ i \in \text{c}. \qquad \text{(hermitean form)} \tag{7}$$

To obtain hermitean form of the equations, we have used the equality $\rho |\psi_i\rangle = |\psi_i\rangle$ which is valid for occupied states but not for vacant ones.

2.2. PROPERTIES OF "PSEUDOPROJECTORS"

In our earlier works [17, 18] we have shown as follows – operators P_c and P_r
a) are idempotent

$$\left(P_c\right)^2 = P_c, \left(P_r\right)^2 = P_r;$$

b) are invariant with respect to linear transformation of the cluster states;
c) are invariant with respect to linear transformation of the remaining system states, too;
d) may be decomposed on projectors and rotation operators.

Consider the latter property more detailed. Because the cluster and the remaining system wave functions are linearly independent, without loss of generality the wave functions of the cluster may be expressed as

$$|\psi_i\rangle = |\phi_i\rangle + \sum_{j\in r} |\varphi_j\rangle a_{ji}, \ i \in \text{c}, \tag{8}$$

where

$|\phi_i\rangle$, $i \in$ c, are linearly independent but in general are not orthogonal to each other, $\langle \phi_i | \phi_j \rangle = B_{ij}$;

$|\varphi_j\rangle$, $j \in$ r, are not mutually orthogonal, too,

$\langle \varphi_i | \varphi_j \rangle = (S_r)_{ij}$;

while $|\phi_i\rangle$, $i \in$ c, are orthogonal to $|\varphi_j\rangle$, $j \in$ r, $\langle \phi_i | \varphi_j \rangle = 0$.

Substituting expansion (8) in the definitions of operators P_c and P_r (formulas (4) and (5)) and using results of Appendix we finally get:

$$P_c = \sum_{i,j \in c} |\phi_i\rangle (B^{-1})_{ij} \langle \phi_j | + \sum_{i \in r} \sum_{j \in c} |\varphi_i\rangle (A_c B^{-1})_{ij} \langle \phi_j |, \tag{9}$$

$$P_r = \sum_{i,j \in r} |\varphi_i\rangle (S_r^{-1})_{ij} \langle \varphi_j | - \sum_{i \in r} \sum_{j \in c} |\varphi_i\rangle (A_c B^{-1})_{ij} \langle \phi_j |. \tag{10}$$

Matrix A_c is matrix of coefficients a_{ji} in expansion (8) for the cluster wave functions.

First terms in the expressions (9) and (10) are projection operators, while second ones are rotation operators. Projector in expression (10) is projector on the remaining system wave functions space Ω_r

$$\Omega_r = \sum_{i,j \in r} |\varphi_i\rangle (S_r^{-1})_{ij} \langle \varphi_j |, \tag{11}$$

where S_r is the matrix of the remaining system spin-orbital overlaps.

Denote projector in (9) as

$$W_c = \sum_{i,j \in c} |\phi_i\rangle (B^{-1})_{ij} \langle \phi_j |. \tag{12}$$

Defining rotation operator R_c as

$$R_c = \sum_{i \in r} \sum_{j \in c} |\varphi_i\rangle (A_c B^{-1})_{ij} \langle \phi_j | \tag{13}$$

we may rewrite (9) and (10) in the following way:

$$P_c = W_c + R_c, \tag{14}$$

$$P_r = \Omega_r - R_c. \tag{15}$$

Taking into account that $P_r + P_c = \rho$ it is easy to see that sum of projectors W_c and Ω_r gives one-electron density operator (3) for the whole system:

$$\Omega_r + W_c = \rho.$$

2.3. TRASFORMATION TO AN EIGENVALUE AND EIGENVECTOR PROBLEM

It is easy to see that every linear combination of the solutions of Eqs. (6) is also solution of these equations. We follow ideas of Adams and Gilbert [12-16] and transform our equations to these of eigenvalue and eigenvector task:

$$\left([1-\rho] F P_c^+ + A\right) |\psi_i\rangle = \lambda_i |\psi_i\rangle, \quad i \in \text{c}. \tag{16}$$

In order we get Eqs. (6) like the consequence of Eqs. (16), the following restriction must be imposed on A [17, 18]:

$$\rho A |\psi_i\rangle = A |\psi_i\rangle, \quad i \in \text{c}. \tag{17}$$

If operator A is properly chosen spectral task (16) has non-degenerate linearly independent solutions. We should stress that we have no demanded operator A to be hermitean. Generally speaking, approach of Adams and Gilbert does not require consideration of eigenvalue and eigenvector problem for hermitean operator. To pass from homogeneous equations to eigenvalue equations, instead of Adams-Gilbert construction $\rho A \rho$ it is sufficient to consider operator A satisfying condition (17).

2.4. THE CASE OF MUTUALLY ORTHOGONAL CLUSTER WAVE FUNCTIONS

For practical applications it is important to consider the case when cluster one-electron wave functions are mutually orthogonal but stay to be not orthogonal to the remaining system one-electron wave functions. (It is the standard situation treated in the theory of pseudopotentials [23].) To get mutually orthogonal solutions we must obtain eigenvalue and eigenvector problem for hermitean operator with non-degenerate spectrum. Homogeneous equations may be written in hermitean form (7), so we may choose $A = P_c(F+G)P_c^+$ (it is easy to prove that restriction (17) is valid for this A):

$$\left(\left[1-P_r\right]F\left[1-P_r\right]^+ + P_c G P_c^+\right)\left|\psi_i\right\rangle = E_i\left|\psi_i\right\rangle,\ i\in\mathrm{c}, \tag{18}$$

where G is hermitean operator.

In the theory of pseudopotentials [23] not only wave functions of the varied subsystem, but also those of the frozen subsystem are solutions of the equations. In our earlier work [18] we have shown that if operator G is properly chosen wave functions of the rest of system are not solutions of our Eqs. (18) with the exception of the case when we demand the wave functions of the cluster to be orthogonal to those of the rest of system.

If we choose $G=0$ we get the following equations:

$$\left(1-P_r\right)F\left(1-P_r^+\right)\left|\psi_i\right\rangle = E_i\left|\psi_i\right\rangle,\ \ i\in\mathrm{c}. \tag{19}$$

These equations coincide with those obtained by H. Stoll et al. [22]. They present not general, but very important case of equations for mutually orthogonal cluster wave functions. In our previous work [18] we have shown that after imposing orthogonality restrictions on the wave functions Eqs. (19) convert to well-known equations of Huzinaga [5, 6]. Eqs. (18) require more general further investigation.

Ascertain that solutions of Eqs. (18) really are not orthogonal to the remaining system wave functions. Acting on both sides of (18) by previously defined projector on the remaining system states Ω_r (see formula (11)) we obtain

$$\left(\Omega_r\left[1-P_r\right]F\left[1-P_r\right]^+ + \Omega_r P_c G P_c^+\right)\left|\psi_i\right\rangle = E_i\Omega_r\left|\psi_i\right\rangle,\ \ i\in\mathrm{c}.$$

Because $\Omega_r\left(1-P_r\right)=\Omega_r\left(1-\Omega_r+R_c\right)=R_c$ and $\Omega_r P_c=\Omega_r\left(W_c+R_c\right)=R_c$ (see formulas from (9) to (15)) we get

$$R_c\left(F\left(1-P_r^+\right)+GP_c^+\right)\left|\psi_i\right\rangle = E_i\Omega_r\left|\psi_i\right\rangle,\ \ i\in\mathrm{c}.$$

Operator in the left side of this equation never turns to zero (except the case when $R_c=0$). So, the right side is not zero, too. It means that $\Omega_r\left|\psi_i\right\rangle\neq 0$ and solutions of Eqs. (18) really are not orthogonal to the remaining system one-electron wave functions. Special case when this is not valid ($R_c=0$, $P_r=\Omega_r$) corresponds to additional demanding on the wave functions of the cluster to be orthogonal to those of the rest of system.

Eqs. (18) describe every possible localisation of the cluster wave functions beyond the cluster region [18]. Their solutions are mutually orthogonal but remain to be non-orthogonal to the wave functions of the rest of system.

3. Vacant states

Equations for the cluster wave functions may lead to different structure of their solutions for occupied states and for vacant ones. Study this problem more detailer. Define vacant solutions as extra solutions staying linearly independent with the cluster and the rest of the system occupied states. (According to this definition $\rho|\psi_i\rangle \neq |\psi_i\rangle$, $i\in$v, but not necessarily $\rho|\psi_i\rangle = 0$.)

Solutions of Eqs. (18) are mutually orthogonal because operator in the left part of these equations is hermitean. Being solutions of these equations occupied cluster states and vacant ones are orthogonal to each other. It means that vacant solutions of Eqs. (18) satisfy condition

$$(1-\Omega_c)|\psi_i\rangle = |\psi_i\rangle, \quad i\in\text{v}, \tag{20}$$

where Ω_c is projector on the occupied cluster states,

$$\Omega_c = \sum_{i,j\in c} |\psi_i\rangle (S_c^{-1})_{ij} \langle\psi_j|,$$

S_c is the matrix of the cluster wave functions overlaps.

We may obtain equations for vacant states acting by $(1-\Omega_c)$ on both sides of Eqs. (18). Taking into account properties of ρ, Ω_c, P_r and P_c we have:

$$\Omega_c P_c = P_c, \ (1-\Omega_c)P_c = 0 \ ; \quad \Omega_c \rho = \Omega_c, \ (1-\Omega_c)(1-\rho) = (1-\rho);$$

$$P_r = \rho - P_c,$$

$$(1-\Omega_c)(1-P_r) = (1-\Omega_c)[(1-\rho)+P_c] = (1-\rho). \tag{21}$$

Therefore, acting by $(1-\Omega_c)$ on both sides of Eqs. (18) we get

$$(1-\rho)F(1-P_r^+)|\psi_i\rangle = E_i(1-\Omega_c)|\psi_i\rangle, \ i\in\text{v}.$$

Taking condition (20) into account and using (21) we have:

$$(1-P_r^+)|\psi_i\rangle = (1-P_r^+)(1-\Omega_c)|\psi_i\rangle = [(1-\Omega_c)(1-P_r)]^+|\psi_i\rangle = (1-\rho)|\psi_i\rangle, \quad i\in\text{v}.$$

Summing up these results, we see that vacant solutions of Eqs. (18) and (19) satisfy the following equations:

$$(1-\rho)F|\psi_i\rangle = E_i|\psi_i\rangle, \ i\in\text{v}. \tag{22}$$

It means that vacant solutions of Eqs. (19) and more general Eqs. (18) are canonical Hartree-Fock orbitals known to be delocalised over the whole system. They are orthogonal to the occupied states both of the cluster and of the rest of system. Operator $(1-\rho)$ in the left side ensures this orthogonality.

If we want vacant solutions to be localised in the same way as occupied cluster states we should modify our equations. To get occupied and vacant solutions of the similar structure we need equations causing admixture of the frozen subsystem wave functions in the both occupied and vacant solutions for the system under variation (cluster) as it is described by expansion (8). To ensure vacant and occupied states separation we demand that in the expression of the form (8)

$$\langle\phi_i|\phi_j\rangle = 0, \ i\in\text{c}, \ j\in\text{v}. \tag{23}$$

As long as wave functions $|\phi_i\rangle$, $i\in$v, make our basis complete, result of action $|\chi\rangle = F\left(1-P_r^+\right)|\xi\rangle$ of operator $F\left(1-P_r^+\right)$ on arbitrary wave function may be represented as

$$|\chi\rangle = \sum_{j\in c+v}|\phi_j\rangle c_j + \sum_{j\in r}|\varphi_j\rangle\tilde{c}_j\,. \tag{24}$$

Taking into account (24), (15), (11) and (13) we see that operator $(1-P_r)F\left(1-P_r^+\right)$ acts on arbitrary wave function as follows:

$$(1-P_r)F\left(1-P_r^+\right)|\xi\rangle = (1-P_r)|\chi\rangle = (1-P_r)\left[\sum_{j\in c+v}|\phi_j\rangle c_j + \sum_{j\in r}|\varphi_j\rangle\tilde{c}_j\right] =$$

$$= \left(\left[1-\Omega_r\right]+R_c\right)\left[\sum_{j\in c+v}|\phi_j\rangle c_j + \sum_{j\in r}|\varphi_j\rangle\tilde{c}_j\right] = \sum_{j\in c+v}|\phi_j\rangle c_j + \sum_{j\in c}\sum_{k\in r}|\varphi_k\rangle a_{kj}c_j\,.$$

The latter sum contains admixture of the remaining system wave functions for the cluster occupied states and not for vacant ones. It is the reason why occupied and vacant solutions of Eqs. (19) have different structure.

By analogy with rotation operator R_c for occupied cluster states define rotation operator for vacant states R_v as

$$R_v = \sum_{j\in r}\sum_{k\in v}|\varphi_j\rangle\left(A_v D^{-1}\right)_{jk}\langle\phi_k|\,, \tag{25}$$

where $|\varphi_j\rangle$, $j\in$r, $|\phi_k\rangle$, $k\in$v, are wave functions and A_v is matrix of coefficients a_{ji} in expansion of form (8) for vacant solutions;

$$D_{ij} = \langle\phi_i|\phi_j\rangle,\ i,j\in\text{v};$$

$|\phi_k\rangle$, $k\in$v, belong to orthogonal to both cluster and the rest of system occupied wave functions space, $\langle\phi_i|\phi_k\rangle = 0$, $\langle\varphi_j|\phi_k\rangle = 0$, $i\in$c, $j\in$r, $k\in$v.

In addition to rotation operator R_v define operators W_v and P_v by analogy with operators W_c and P_c (see formulas (9)-(14)):

$$W_v = \sum_{i,j\in v}|\phi_i\rangle\left(D^{-1}\right)_{ij}\langle\phi_j|\,, \tag{26}$$

$$P_v = W_v + R_v\,. \tag{27}$$

Substituting (25) and (26) into (27) we get

$$P_v = \sum_{i,j\in v}|\phi_i\rangle\left(D^{-1}\right)_{ij}\langle\phi_j| + \sum_{i\in r}\sum_{j\in v}|\varphi_i\rangle\left(A_v D^{-1}\right)_{ij}\langle\phi_j|\,. \tag{28}$$

Operators R_c and R_v (see their definitions (13) and (25)) have the following properties:

$$R_c\left|\varphi_i\right\rangle = 0,\ i\in\text{r}, \qquad R_c\left|\phi_i\right\rangle = 0,\ i\in\text{v}, \qquad R_c\left|\phi_i\right\rangle = \sum_{j\in r}\left|\varphi_j\right\rangle a_{ji},\ i\in\text{c};$$

$$R_v\left|\varphi_i\right\rangle = 0,\ i\in\text{r}, \qquad R_v\left|\phi_i\right\rangle = 0,\ i\in\text{c}, \qquad R_v\left|\phi_i\right\rangle = \sum_{j\in r}\left|\varphi_j\right\rangle a_{ji},\ i\in\text{v};$$

$$\text{while } \left(R_c + R_v\right)\left|\phi_i\right\rangle = \sum_{j\in r}\left|\varphi_j\right\rangle a_{ji},\ i\in\text{c+v}. \tag{29}$$

Therefore, to get the same structure of occupied and vacant solutions, we may modify Eqs. (19) replacing operator $\left(1-P_r\right)$ by operator $\left(1-\Omega_r\right)+R_c+R_v$:

$$\left(\left[1-\Omega_r\right]+R_c+R_v\right)F\left(\left[1-\Omega_r\right]+R_c^+ + R_v^+\right)\left|\psi_i\right\rangle = E_i\left|\psi_i\right\rangle,\ i\in\text{c+v}. \tag{30}$$

If we want Eqs. (30) and Eqs. (19) to have the same solutions for the cluster occupied states on one hand we have to demand that

$$R_v^+\left|\psi_i\right\rangle = 0,\ i\in\text{c}.$$

On the other hand, taking into account expansion (8) for the cluster wave functions and definition (25) of operator R_v we get

$$R_v^+\left|\psi_i\right\rangle = \sum_{j\in v}\left|\phi_j\right\rangle\left(D^{-1}A_v^+ S_r A_c\right)_{ji},\ i\in\text{c}.$$

Therefore, we should impose the following restriction $A_v^+ S_r A_c = 0$ or its hermitean conjugate

$$A_c^+ S_r A_v = 0.$$

It is easy to prove that under this restriction $\Omega_c R_v = 0$. As the result, Eqs. (30) and Eqs. (19) have the same solutions for the cluster occupied states.

Establish general structure of the solutions of Eqs. (30). If we consider that cluster states $\left|\psi_i\right\rangle$ are described by expansion (8) then

$$\left(1-\Omega_r\right)\left|\psi_i\right\rangle = \left|\phi_i\right\rangle,\ i\in\text{c+v},$$

$$\left(R_c^+ + R_v^+\right)\left|\psi_i\right\rangle = \begin{cases} \sum_{j\in c}\left|\phi_j\right\rangle\left(B^{-1}A_c^+ S_r A_c\right)_{ji}, i\in\text{c} \\ \sum_{j\in v}\left|\phi_j\right\rangle\left(D^{-1}A_v^+ S_r A_v\right)_{ji}, i\in\text{v}. \end{cases}$$

It means that operator $\left(1-\Omega_r\right)+R_c^+ + R_c^+$ does not mix occupied and vacant states with each other.

Result of action $\left|\chi\right\rangle = F\left(\left[1-\Omega_r\right]+R_c^+ + R_c^+\right)\left|\xi\right\rangle$ of operator $F\left(\left[1-\Omega_r\right]+R_c^+ + R_c^+\right)$ on arbitrary wave function without loss of generality may be expressed by formula (24); then the left side of Eqs. (30) gives wave function of the following structure:

$$\left(\left[1-\Omega_r\right]+R_c+R_v\right)\left|\chi\right\rangle = \sum_{j\in c+v}\left|\phi_j\right\rangle c_j + \sum_{j\in c+v}\sum_{k\in r}\left|\varphi_k\right\rangle a_{kj}c_j.$$

We see that unlike our initial equations (19) modified equations (30) give admixture of the remaining system wave functions for both occupied and vacant cluster states. So, solutions of modified equations (30) have the same structure and therefore the same degree of localisation for both occupied and vacant cluster states. For occupied cluster states solutions of these equations are the same as those of our initial equations (19). Due to these two reasons Eqs. (30) may be used as starting equations for one of the existing methods including many-electron correlation effects into consideration.

4. Summary and conclusions

We have treated problem "cluster in the field of the remaining part of system" by direct variational approach. Our consideration is general for every task "subsystem in the field of the frozen remaining part of the whole system" (cluster and the rest of crystal, fragment of a molecule and the remaining part of it, valence and core electrons, etc.).

Total energy of the whole system (cluster + the rest of system) is expressed in terms of non-orthogonal one-electron wave functions. Equations for the cluster wave functions are obtained from variation of the total energy expression subject to the condition that wave functions of the rest of system are known and fixed. Mutual orthogonality restrictions are not imposed. Equations for non-orthogonal wave functions are variational equations.

We have shown that general (homogeneous) equations (describing linear space of the cluster wave functions) may be transformed to the eigenvalue and eigenvector problem equations (selecting basis for this space). We have proposed equations for mutually orthogonal cluster wave functions keeping them to be not orthogonal to the wave functions of the remaining system. We have found that the remaining system wave functions are not solutions of these equations. Possibility to formulate task so that remaining system wave functions do not appear as solutions of the equations for the cluster seems to be a significant advantage of our approach.

We have studied vacant solutions of our equations. We have found that vacant solutions of our initial equations are canonical Hartree-Fock orbital delocalised over the whole system; while occupied solutions are localised in the cluster region. It limits further applications of EMC model because it does not allow us to go beyond one-electron approximation. Any of existing methods including many-electron correlation effects into consideration require both vacant and occupied electron states to have the same degree of localisation. Besides that, when occupied states are well-localised while vacant ones stay to be delocalised it becomes impossible to calculate optical transition energies and magnetic resonance effects in the frameworks of one-electron approximation with frozen electron states.

We have demonstrated that proposed in our earlier work [18] projection and rotation operator technique give us possibility to overcome these limitations. We have shown that it is possible to modify our initial equations in such a way that their vacant solutions have the same degree of localisation as occupied ones. It gives us opportunity to go beyond one-electron approximation and to include many-electron correlation effects into consideration.

References

[1] Pisani C. (1978) Approach to the embedding problem in chemisorption in a self-consistent-field molecular-orbital formalism. *Phys. Rev. B* **17**, 3143-3153.

[2] Pisani C., Dovesi R. and Carosso P. (1979) Moderately-large-embedded-cluster approach to the study of local defects in solids. Vacancy and substitutional impurity in graphite. *Phys. Rev. B* **20**, 5345-5357.

[3] Pisani C., Dovesi R., Nada R. and Kantorovich L. N. (1990) Ab initio Hartree-Fock perturbed cluster treatment of local defects in crystals. *J. Chem. Phys.* **92**, 7448-7460.

[4] Kantorovich L. N. (1988) An embedded-molecular-cluster method for calculating the electronic structure of point defects in non-metallic crystals. I. General theory. *J. Phys. C: Solid State Phys.* **21**, 5041-5056. An embedded-molecular-cluster method for calculating the electronic structure of point defects in non-metallic crystals. II. Structural elements in a form of molecules. *J. Phys. C: Solid State Phys.* **21**, 5057-5073.

[5] Huzinaga S. and Cantu A. A. (1971) Theory of separability of many-electron systems. *J. Chem. Phys.* **55**, 5543-5549.

[6] Huzinaga S., Mc Williams D. and Cantu A. A. (1973) Projection operators in Hartree-Fock theory. *Adv. Quantum Chem.* **7**, 187-220.

[7] Barandiaran Z. and Seijo L. (1988) The ab initio model potential representation of the crystalline environment. Theoretical study of the local distortion on NaCl:Cu^+. *J. Chem. Phys.* **89**, 5739-5746.

[8] Seijo L. and Barandiaran Z. (1992) Self-consistent embedded clusters: building block equations for localized orthogonal orbitals. *J. Math. Chem.* **10**, 41-56.
[9] Seijo L. and Barandiaran Z. (1996) Application of the group-function theory to the field of materials science. *Int. J. Quantum Chem.* **60**, 617-634.
[10] Mejias J. A. and Sanz J. F. (1995) Compact model potentials for ab initio embedded cluster calculations. Part I. Basic Formulation. *J. Chem. Phys.* **102**, 327-336. Unrestricted compact model potentials for ab initio embedded cluster calculations: Magnetic interactions in $KNiF_3$. *J. Chem. Phys.* **102**, 850-858.
[11] Anderson P. W. (1968) Self-consistent pseudopotentials and ultra-localized functions for energy bands. *Phys. Rev. Lett.* **21**, 13-16.
[12] Adams W. H. (1961) On the solution of the Hartree-Fock equation in terms of localized orbitals. *J. Chem. Phys.* **34**, 89-102.
[13] Adams W. H. (1962) Orbital theories of electronic structure. *J. Chem. Phys.* **37**, 2009-2018.
[14] Adams W. H. (1965) Orbital theories of electronic structure. II. Molecularly invariant orbitals. *J. Chem. Phys.* **42**, 4030-4038.
[15] Gilbert T. L. (1964) Self-consistent equations for localized orbitals in polyatomic systems. In: *Molecular Orbitals in Chemistry, Physics and Biology*. New York and London: Academic Press, 405-420.
[16] Gilbert T. L. (1974) Selection of self-consistent-field orbitals. *J. Chem. Phys.* **60**, 1789-1791.
[17] Shidlovskaya E. K. (1996) Rigorous approach to the construction of pseudopotential from crystalline environment in embedded molecular cluster model. *Latvian Journal of Physics and Technical Sciences*, No. 4, 57-82.
[18] Shidlovskaya E. K. (2002) Improved embedded molecular cluster model. *Int. J. Quantum Chem.* **89**, 349-370.
[19] Löwdin P.-O. (1950) On the non-orthogonality problem connected with the use of atomic wave functions in the theory of molecules and crystals. *J. Chem. Phys.* **18**, 365-375.
[20] Löwdin P.-O. (1955) Quantum theory of many-particle systems. II. Study of the ordinary Hartree-Fock approximation. *Phys. Rev.* **97**, 1490-1508.
[21] Stoll H., Wagenblast G. and Preuss H. (1978) On the Hartree-Fock theory of local regions in molecules. *J. Am. Chem. Soc.* **100**, 7742-7743.
[22] Stoll H., Wagenblast G. and Preuss H. (1980) On the use of local basis sets for localized molecular orbitals. *Theor. Chem. Acta* **57**, 169-178.
[23] Szasz L. (1985) *Pseudopotential Theory of Atoms and Molecules.* New York: John Wiley.

Appendix

When we divide quantum system on two subsystems (cluster and the rest of system in our case) matrix of one-electron wave functions overlaps and its inverse may be written in the block form:

$$S = \begin{pmatrix} S_c & S_{cr} \\ S_{rc} & S_r \end{pmatrix}, \qquad S^{-1} = Q = \begin{pmatrix} Q^c & Q^{cr} \\ Q^{rc} & Q^r \end{pmatrix}.$$

According to the definition of the inverse matrix, $QS = I$, where I is the unity matrix. Write this equality in the block form:

$$Q^c S_c + Q^{cr} S_{rc} = I_c, \quad \text{(A1)} \qquad Q^c S_{cr} + Q^{cr} S_r = 0, \quad \text{(A2)}$$

$$Q^{rc} S_c + Q^r S_{rc} = 0, \quad \text{(A3)} \qquad Q^{rc} S_{cr} + Q^r S_r = I_r. \quad \text{(A4)}$$

From (A2) and (A3) we obtain

$$Q^{cr} = -Q^c S_{cr} S_r^{-1}, \quad \text{(A5)} \qquad Q^{rc} = -Q^r S_{rc} S_c^{-1}. \quad \text{(A6)}$$

Substituting (A5) into (A1) we come to

$$Q^c S_c - Q^c S_{cr} S_r^{-1} S_{rc} = I_c.$$

Therefore

$$Q^c = \left(S_c - S_{cr} S_r^{-1} S_{rc}\right)^{-1}. \quad \text{(A7)}$$

In the similar way, substituting (A6) into (A4), we obtain

$$Q^r = \left(S_r - S_{rc} S_c^{-1} S_{cr}\right)^{-1}. \quad \text{(A8)}$$

On the other hand, according to the definition of the inverse matrix, $SQ = I$. Write this equality in the block form:

$$S_c Q^c + S_{cr} Q^{rc} = I_c, \qquad S_c Q^{cr} + S_{cr} Q^r = 0, \qquad \text{(A9)}$$

$$S_{rc} Q^c + S_r Q^{rc} = 0, \qquad \text{(A10)} \qquad S_{rc} Q^{cr} + S_r Q^r = I_r.$$

From (A9) and (A10) we obtain

$$Q^{cr} = -S_c^{-1} S_{cr} Q^r, \qquad \text{(A11)} \qquad Q^{rc} = -S_r^{-1} S_{rc} Q^c. \qquad \text{(A12)}$$

Substituting (A11) into (A1) we have

$$Q^c S_c - S_c^{-1} S_{cr} Q^r S_{rc} = I_c.$$

Therefore

$$Q^c = S_c^{-1} + S_c^{-1} S_{cr} Q^r S_{rc} S_c^{-1}. \qquad \text{(A13)}$$

In a similar way, substituting (A12) into (A4) we get

$$Q^r = S_r^{-1} + S_r^{-1} S_{rc} Q^c S_{cr} S_r^{-1}. \qquad \text{(A14)}$$

Collecting these results we finally have

$$Q^c = \left(S_c - S_{cr} S_r^{-1} S_{rc}\right)^{-1} = S_c^{-1} + S_c^{-1} S_{cr} Q^r S_{rc} S_c^{-1};$$

$$Q^{cr} = -Q^c S_{cr} S_r^{-1} = -S_c^{-1} S_{cr} Q^r;$$

$$Q^{rc} = -Q^r S_{rc} S_c^{-1} = -S_r^{-1} S_{rc} Q^c;$$

$$Q^r = \left(S_r - S_{rc} S_c^{-1} S_{cr}\right)^{-1} = S_r^{-1} + S_r^{-1} S_{rc} Q^c S_{cr} S_r^{-1}.$$

Consider wave functions of the cluster, which are linearly independent with those of the frozen rest of our system. Without loss of generality they may be expressed as

$$\left|\psi_i\right\rangle = \left|\phi_i\right\rangle + \sum_{j \in r} \left|\varphi_j\right\rangle a_{ji}, \quad i \in \mathrm{c}, \qquad \text{(A15)}$$

where

$\left|\phi_i\right\rangle$ are linearly independent but in general are not orthogonal to each other, $\left\langle \phi_i \middle| \phi_j \right\rangle = B_{ij}$;

wave functions of the rest of system $\left|\varphi_j\right\rangle$, $j \in$ r, are not mutually orthogonal, too, $\left\langle \varphi_i \middle| \varphi_j \right\rangle = \left(S_r\right)_{ij}$;

while $\left|\phi_i\right\rangle$ are orthogonal to the wave functions of the rest of system $\left|\varphi_j\right\rangle$, $\left\langle \phi_i \middle| \varphi_j \right\rangle = 0$.

Using this expansion, we get the following expressions for the wave functions overlap matrix S for our system (cluster + the rest of system):

$$S = \begin{pmatrix} S_c & S_{cr} \\ S_{rc} & S_r \end{pmatrix} = \begin{pmatrix} B + A^+ S_r A & A^+ S_r \\ S_r A & S_r \end{pmatrix}, \qquad \text{(A16)}$$

where A is matrix of coefficients a_{ji} in the expansion (A15) for the cluster wave functions.

For the inverse matrix $Q = S^{-1}$, substituting (A16) into the formulas (A7), (A5), (A12) and (A14), we have finally

$$S^{-1} = Q = \begin{pmatrix} Q^c & Q^{cr} \\ Q^{rc} & Q^r \end{pmatrix} = \begin{pmatrix} B^{-1} & -B^{-1} A^+ \\ -AB^{-1} & S_r^{-1} + AB^{-1} A^+ \end{pmatrix}. \qquad \text{(A17)}$$

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NEW APPROACH IN *AB INITIO* DESCRIPTION OF ION BEAM INDUCED PHASE TRANSFORMATIONS

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Ab initio calculations are performed to study the phase transitions in Mg alloys induced by Plasma Immersion Ion Implantation (PIII). It was proposed a new approach for prediction of the formation of new phases based of the analysis of electronic characteristics of the intermediate state which is formed in the beginning of the ion induced phase transition. The mechanism of the formation of new structure Mg-28.35.at %.Al-18.34 at %Ag was found.

Keywords: *phase transformations, ion implantation, Mg alloys*

1. Introduction

Radiation resistance of materials is the main problem in radiation physics. Studies of radiation-stimulated processes in solids are devoted usually to elucidation of mechanisms of radiation destruction of materials. The interpretation of results is based on the consideration of material parameters linked to the initial crystal structure [1], electro-negativities [2] of alloy constituents or specific features of phase diagram [3]. A lot of theoretical results are obtained by molecular dynamics (MD) simulation. This approach is applied both to pure elements and to alloys [4, 5]. One of the important fields in radiation physics is the radiation-stimulated modification of materials and improvement of their service characteristics. In spite of the long history of investigations of radiation-stimulated processes the necessary understanding of microscopic mechanisms of the radiation-induced changes in electronic and in lattice subsystems in solids is not achieved yet.

Nowadays a wide application of Plasma Immersion Ion Implantation and Deposition (PI^3&D) led to new promising feasibilities of the radiation modification of solid surfaces and creation of novel materials. The experimental results show that new types of compounds and new structural types can be produced using PI^3&D [6]. These results lead to important applications of PI^3&D and may be used as a basis for theoretical studies of mechanisms of ion beam induced processes in solid surfaces. The difficulties of theoretical studies of these processes based on *ab initio* approach are caused by necessity to deal with strongly in-harmonic and non-adiabatic systems. As a rule we have detailed information about structural and electronic characteristics for materials before irradiation and do not have the corresponding information for irradiated materials. New structures and compounds that are obtained as a result of PI^3&D treatment of well-known materials are often demand large efforts for their identification and studies. Therefore the important problem is a development of the adequate theoretical approach for prediction of radiation-induced changes of materials proceeding from the properties of non-irradiated materials and using the corresponding models of radiation processes.

In [7] we suggested the existence of *a correlation between the final structural characteristics of the new ion-induced phase and the electronic properties of the old phase at the first stage of the ion-induced process.* This intermediate state (IS) corresponds to strongly non-equilibrium characteristics of material. We assume that in IS the implanted ions are already inside the crystal but any phase transformations of the system still did not occur. This model is based on the adiabatic approximation: the appearance of implanted ions in the host lattice leads to "immediate" excitation of the electronic subsystem of the crystal while the transformations of atomic configurations will occur later. The reconstruction of atomic configurations and the formation of new phases is the next stage of the radiation-induced process. As a matter of fact IS is not visible state of material. But our *ab initio* studies showed that it is possible to predict fact that the formation of new phase begins in the bowels of the old phase from the reconstruction of the electronic subsystem. We show that *ab initio* studies of IS of material in the radiation-induced process are useful for prediction the composition of new radiation-induced phase.

In this paper we report the results of further the radiation conditions of the formation of new phases analyzing the electronic characteristics of materials in IS, i.e. at the first stage of irradiation. In particular the concentration dependence of these parameters serves as a factor for predicting the formation of new phase. Our approach is based on the development of approach described in [7]. The subject of investigation is a system Mg-Al-Ag that is obtained by implantation of Ag ions into Mg-Al alloy. Experimental results show that at some concentration of implanted Ag ions in conditions of PI^3&D a formation of new unknown phase takes place. Our theory allows predict the atomic fraction of implanted Ag ions, z, and hence the retained dose of implanted ions that leads to the formation of the new phase. The experimental procedure and results are presented in Section 2. In Section 3 we describe the developed approach for the general case of formation of the compound with arbitrary composition $Mg_xAl_yAg_{1-x-y}$ and apply it to study the new structural type that was found experimentally. In Section 4 we discuss the obtained results.

2. Experimental results

The commercial magnesium alloy AZ91 of composition Mg-9wt%Al-1wt%Zn-0.3wt%Mn was a target material. In its as-cast condition the alloy contained two main phases: Mg matrix and large grains of the so-called beta phase, which is an inter-metallic compound with the nominal composition $Mg_{17}Al_{12}$. This phase has a cubic unit cell with the parameter a = 1.05438 nm and can be described by the space group $I\bar{4}3m$.

TEM examination of the implanted beta particles revealed that their structure has been changed: instead of binary cubic beta phase an unknown ternary phase was formed with the approximate composition Mg-28.35.at%.Al-18.34 at%Ag, as it was determined by energy-dispersive x-ray microprobe analysis. Attempts to identify the structure of this phase on the basis of the ternary phases known in the literature for the Mg-Al-Ag system were unsuccessful; therefore, we performed a structural study of the new phase.

For the determination of the unit cell parameters and type of Bravais lattice a number of conventional selected area diffraction patterns were taken in the electron microscope. It turned out that all patterns could be indexed on the basis of cubic unit cell with the lattice parameters a = 2.03nm.

A detailed analysis of electron diffractions has shown that all observed reflections obey the condition h + k = 2n and h + l = 2n and k + l = 2n, thus indicating that the Bravais lattice describing the new structure can only be of face-centred (F) type.

The point group of the new ternary phase was determined by the electron-micro-diffraction technique based on analysis of the symmetry of zero-order (ZOLZ) and first-order (FOLZ) Laue zones. It was obtained that the point group describing the new phase should be chosen as $m\bar{3}m$.

3. The model and calculation details

The experimental results showed that the new phase $Mg_{0.53}Al_{0.28}Ag_{0.19}$ is formed as a result of PI^3&D treatment of the β-phase of the Mg-Al alloy. Using *ab initio* calculations we study the changes that occur in this phase when different amounts of Ag atoms are added.

The unit cell of β-phase consists of 58 atoms (34 atoms of Mg and 24 atoms of Al). For each concentration of implanted Ag ions we determine the number of Ag atoms x_1 substituting for Mg atoms and y_1 for Al atoms. This can be done proceeding from the requirement that the stoichiometric ratio of elements inherent to the given compound $Mg_xAl_yAg_{1-x-y}$ has to be satisfied. Thus we obtain equations to find x_1 and y_1 for each z:

$$\frac{34-x_1}{24-y_1}=\frac{x}{y};\ \frac{34-x_1}{58}+\frac{24-y_1}{58}+z=1. \qquad (1)$$

Next, we calculate the dependence of the total energy, E_{tot} of the system on z as in the Ref. [7].

Ab initio calculations were carried out using linear muffin-tin orbital (LMTO) method in atomic sphere approximation (ASA) [8]. The important ingredients of this approach are volume- and energy-independent structure constants, and parameters, which contain information relating to the one-electron potential. These quantities completely specify the band structure of a given material in a given crystal structure. This description is valid for closely packed crystalline solids and gives a physically simple picture of energy bands formation. The computer program, which was used, accounts multipole corrections to ASA and transfer effects in the coherent potential approximation (CPA) [13]. The last

approximation is involved in calculations when Ag atoms are added to β–phase. With self-consistently obtained bands the program calculates the total energies of the system. Core electrons are frozen after initial atomic calculations. For the total energy calculations the convergence criterion was chosen as 0.001 mRy. The calculation details are described in [7].

The total energy, $\boldsymbol{E_{tot}}$ of the β-phase $Mg_{17}Al_{12}$ was calculated for a set of lattice parameters in vicinity of the experimental value, a = 10.5 Å. The results of these calculations are presented in Table1.

TABLE 1. Total energy, $\boldsymbol{E_{tot}}$ in the region of the variation ofWigner-Seitz radius, R_{WZ}, and the corresponding lattice parameter, $\boldsymbol{a}$

N°	R_{WZ}, Å	$\boldsymbol{a}$, Å	$\boldsymbol{E_{tot}}$, Ry
1	3.08	10.17	-434.1271982
2	3.10	10.23	-434.0925950
3	3.11	10.27	-434.1168390
4	3.12	10.30	-434.1344382
5	3.15	10.40	-434.1279328
6	3.17	10.46	-434.1135584
7	3.18	10.50	-434.1033576

One can see that the minimal value of $\boldsymbol{E_{tot}}$ (the fourth line in Table 1) is close to experimental value of lattice parameter for the β-phase of the Mg-Al alloy. It means that the chosen method and computer program are suitable for the further study of this system.

On the next stage we calculated the electronic parameters of β-phase with Ag atoms that substitute for Mg and Al atoms according to above formulated conditions (1). The total energy, $\boldsymbol{E_{tot}}$ and the Densities of States for electrons (DOS) were calculated for different $\boldsymbol{z}$ in (1) and consequently for some range of retained doses of implanted ions of Ag. The steps of investigation were as follows: a) For each atomic fraction, z of Ag in $Mg_{0.53}Al_{0.28}Ag_{0.19}$ with the crystal structure of β-phase we found corresponding values of x_1 and y_1 of Ag atoms substituting for different Mg and Al atoms; b) For each z we minimized the total energy of the system with respect to the lattice parameter in order to find for the given z the quasi-equilibrium lattice parameter and the corresponding minimal value of the total energy.

The conditions (1) yield the minimal atomic fraction, $\boldsymbol{z_{min}}$ of implanted ions of Ag that ensure the necessary ratio of components in the compound $Mg_{0.53}Al_{0.28}Ag_{0.19}$. This value corresponds to $\boldsymbol{z_{min}}$ = 0.15. For example for $\boldsymbol{z}$ = 17 at% we substitute Ag atoms for two Mg atoms and eight Al atoms.

Proceeding from these considerations we studied the changes of electronic characteristics of the Mg-Al-Ag system corresponding to the implantation of β-phase by Ag ions for $\boldsymbol{z}$ = 0.15; 0.17; 0.20; 0.23; 0.25; 0.27 and 0.30. The total and partial DOS referring to the IS state of the β-phase different were calculated for different concentrations of implanted Ag ions (within 15 – 30 at% range). Calculated total DOS-curves for the un-implanted β-phase are shown in Figure 1.

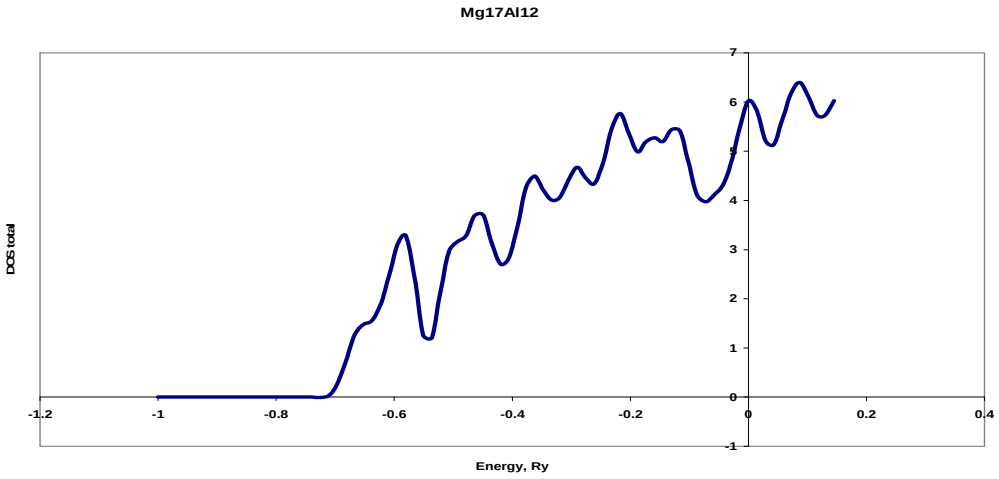

Figure 1. Total DOS calculated for pure β-phase

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In comparison with the un-implanted β-phase the substantial changes of DOS were observed for the concentrations of implanted Ag ions about 17at% and more (Figure 2).

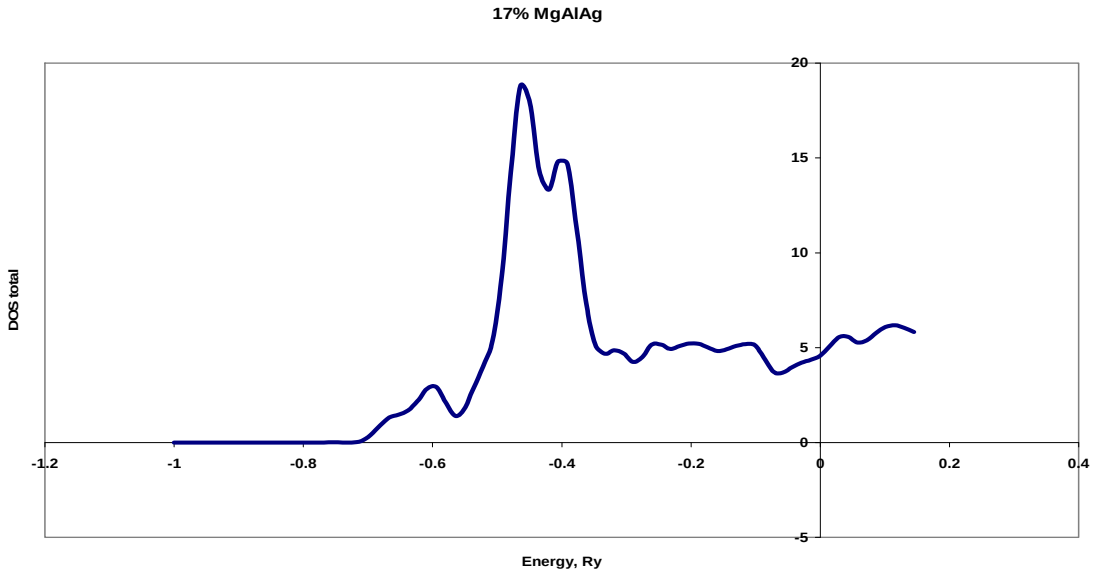

Figure 2. Total DOS calculated for the β-phase implanted by 17 at% of Ag ions

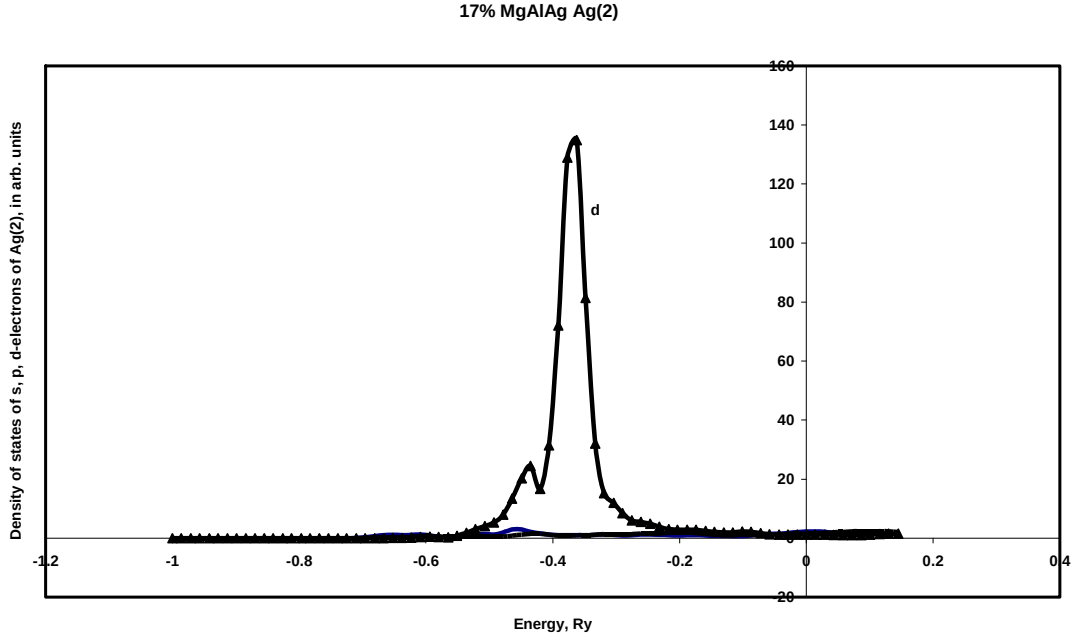

Figure 3. Partial DOS for s, p, and d-electrons of Ag atoms in β-phase implanted by 17 at% Ag

It can be seen in Figures 1 and 2 that for the β-phase implanted by 17 at% Ag the electronic states are located in the narrow region from ~ -0.55 to ~ -0.35 Ry, in comparison with the parent β-phase where the total electronic states are distributed in the wide range -0.7 to + 0.2 Ry.

Referring to Figure 3 showing the partial DOS profiles for *s*, *p* and *d* electrons of Ag atoms in the implanted β-phase we can see that the *d*-states of Ag atoms are dominant being located within the energy range 0.4-0.3Ry, which matches the energy range calculated for total electronic states of implanted β-phase. Fig. 3 shows also that the densities of *s* and *p* states are less of the order of magnitude in comparison with the density of *d* states. It can be concluded, therefore, that in the implanted β-phase *d*-states of Ag atoms are mainly responsible for the profile of the total DOS thus indicating that, when the implanted β-phase transforms to the new structure $Mg_{53}Al_{28}Ag_{19}$, the chemical bonds are formed primarily by *d*-electrons of Ag atoms.

Considering the changes of the partial DOS of Mg atoms we observed that some increase of the density of s-states occurs in the vicinity of -0.4Ry for implanted β-phase. This may imply that, in addition to *d*- electrons of Ag atoms that, apparently, are dominant in the formation of chemical bonds in the new

phase, the *s*-electrons of Mg also contribute to the chemical bonds. Possibly, the effect of *s*-*d* hybridization takes place in this case.

The results concerning the dependence of the features of DOS for implanted β-phase on the concentration of Ag are in line with the results of calculation E_{tot} showing that the increase of E_{tot} occurs within the range from 15 at% to 20 at/% (Figure 4).

4. Discussion

The main question in the problem of the ion beam induced phase formation is what the source of the energy ensures the realization of the corresponding activation processes. The macroscopic temperature in conditions of PI^3&D is low and not enough for the nucleation and growth of the new phase. In [7] it was shown that a mechanism of thermal spikes could be suitable for explanation of experimental results on the low-temperature phase formation under PI^3&D of materials. At present this mechanism is widely used for interpretation of the analogous results [9].

Two important features are revealed as a result of analysis of the dependences of minimal $\boldsymbol{E_{tot}}$ and also the total and partial DOS of the system on the atomic fraction of implanted ions of Ag: a) The conception of the new phase begins for $z > z_{min}$ and therefore demands not only the satisfaction of the stoichiometric formula but also the accumulation of some critical amount of components that ensure the necessary probability of realization of this stoichiometric formula in the given elementary volume; b) The conditions of the new phase formation are saved in some interval of the atomic fraction of Ag.

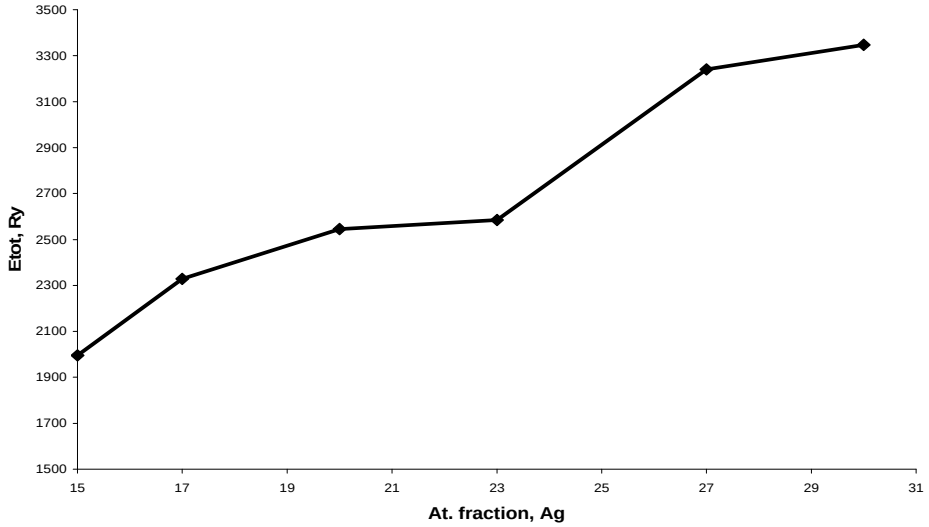

Figure 4. Change in the total energy with concentration of implanted Ag

On the basis of obtained results we conclude *d*-states of Ag and the weak s-d hybridization may be mainly responsible for the formation of chemical bonds in the new phase $Mg_{0.53}Al_{0.28}Ag_{0.19}$.

It is interesting to note that in the case of formation of MgAg compound described in [7] we observed a transformation of *hcp* structure of the initial crystal to the FCC structure of the final phase. In this case *d*-electrons of Ag also played a significant role in formation of the chemical bonds. But these electrons were promoted to s- and p-states with higher symmetry, and this corresponded to formation of the final structure with higher symmetry.

In the case described in this paper the cubic structure of the initial β-phase is preserved after the phase transition and formation of compound $Mg_{0.53}Al_{0.28}Ag_{0.19}$. The results did not show any promotion of electrons with lower symmetry to the states with higher symmetry. The d-electrons of Ag participate directly in the formation of chemical bond in the new phase.

Conclusion

The approach based on the *ab initio* calculations that allow predicting a formation of new phases in conditions of PI^3&D is described. It is shown that calculation of the electronic characteristics of the non-equilibrium IS caused by PI^3&D of materials can be helpful for theoretical prediction of the structural

changes and phase transformations within the implanted matrix. Analysis of the total energy of the system and the total and partial DOS allows finding the retained doses that ensure the corresponding phase transformations. The concentration interval of existence of new phases can be found. The details in the formation of chemical bonds in inter-metallic compound can be also elucidated. The developed approach is applied to understand the mechanism of the formation of new phase $Mg_{0.53}Al_{0.28}Ag_{0.19}$ that is produced by PI^3&D of Ag ions into β-phase of Mg-Al alloy.

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References

[1] Naguib H. M., Kelly R. (1975) *Radiat. Eff.* **25**, 1.
[2] Takayama S. S. (1976) *J. Mater. Sci.* **11**, 164.
[3] Liu B. X. (1987) *Mater. Lett.* **5**, 322.
[4] Van Swygenhoven H., Care A. (1993) *Phys. Rev. Lett.* **70**, 2098.
[5] Diaz de la Rubia T., Averback R. S., Hsieh H., Benedek R. (1989) *J. Mater. Res.* **4**, 579.
[6] Brown Ian G. (1994) Vacuum arc ion sources. *Rev. Sci. Instrum.* **10**, 65.
[7] Kutsenko L., Fuks D., Kiv A., Burlaka L., Talianker M., Monteiro O., Brown I. (2004) *Acta Mat.* **52,** 4329.
[8] Ruban A. V., Skriver H. L. (1999*) Comput. Mater. Sci.* **15**, 119.
[9] Sun Yo., Zhang Ch., Zhu Zh., Wang Zh., Jin Yu., Liu J., and Wang Y. (2004) *Nucl. Instrum. and Methods in Phys. Res. B* **218**, 318.

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INTEGRATED FRAMEWORK FOR SOCIAL, ECONOMIC OR BUSINESS SYSTEM MODELLING

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This paper explores several possible advances in modelling dynamics of complex social, economic or business systems enabled by developments and standardization efforts driven by World Wide Web Consortium and Object Management Group. In particular usage of Meta Object Facility and Semantic Web concepts in connection with System Dynamics modelling technique is presented. Extension mechanism to support collaboration, standardization and reuse of System Dynamics models and their applications is proposed.

Keywords: *complex social, economic business systems, computer modelling*

1. Introduction

The vision that has motivated this work is possibility to develop integrated, widely accessible yet decentralized knowledge base for particular social, economic or other research domain. The main idea is to combine concepts, real world data and models that are related to the domain in to the integrated modelling framework. It's also shown how the framework would enable and facilitate the creation of such knowledge base and how system modelling experts and scientists working in respective research domain could benefit from that. System Dynamics is recognised modelling technique based on General System Theory. It has many applications in environmental disciplines, economic and management sciences, urban planning, energy policy-making etc. It is chosen as preferred modelling language in this paper. However the same framework could support also other modelling techniques. Even more, several modelling languages can be used within the same domain to analyse different problems and still share common vocabulary.

To avoid confusion it should be noted that it is not an attempt to build one all-embracing model for the particular research domain. Such approach probably would be doomed to failure, as some authors have shown it [1]. Instead of that it is proposed that different problems or policies within research domain that are analyzed using particular modelling technique (e.g. System Dynamics) would share common and well-defined vocabulary, utilize and produce structured data. Thus by sharing common domain model effective collaboration, interchange and re-use of models and other knowledge created in modelling process is enabled.

There are number of ways how System Dynamics can be applied in economic and social sciences. However there are not many cases when independent researchers in modelling process would use standardised approach. This makes difficult to benefit from others work. The accumulated knowledge often is dispersed and not structured. The idea's presented here are based on well-established modelling standards driven by Object Management Group [2] which members are virtually all large companies in the computer industry. The other reference group is World Wide Web Consortium [3] that develops interoperable technologies to lead the Internet to its full potential. In particular usage of four layers Meta modelling approach, Meta Object Facility [4], XML and Resource Description Framework [5] concepts is discussed. Paper shows how those standards and technologies together with System Dynamics can be used to create common modelling and knowledge management framework within which complex social, economic or other systems can be explored. Example is provided on how such approach could be used to build interrelated models for Sustainable Human Development studies.

2. Integrated modelling framework

In traditional approach (see Figure 1) systems dynamics models are created to address certain problems within broader social, economic or business context or domain. Such domains themselves are subject of research in respective department of science. From the other hand strategies, a wide range of data supports policies and models that are created in the given environment – it could be measurements

from real world, government accounts, or public inquiries. In this situation the domain concepts and data that are used in model often are not structured and related. Different System Dynamics tools use different dialects of the language and store models in proprietary format that prevents model exchange. Therefore with this approach there are limited possibilities to create synergies when independent modelling efforts are made in the same context or domain.

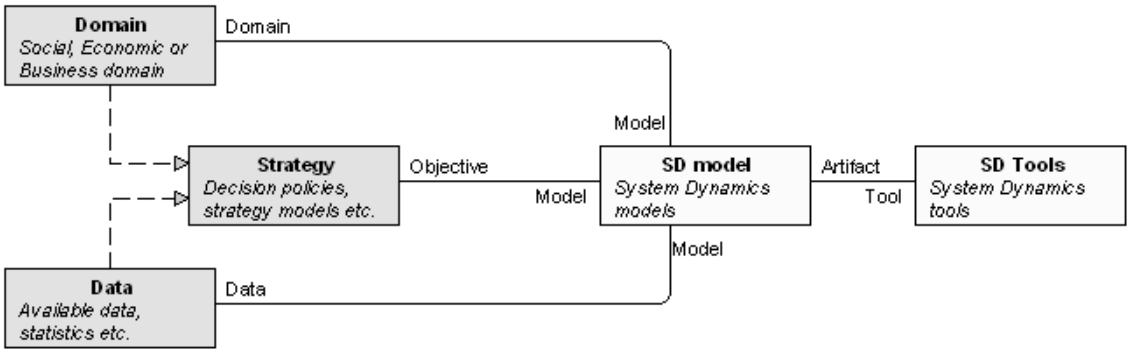

Figure 1. Traditional use of System Dynamics in systems modelling and policy analysis

The main proposal in this paper is to create the integrated modelling framework for respective social, business or economics system (see Figure 2). Meta Object Facility (MOF) is recognised standard for defining metadata therefore it is used here for model notation. By introducing domain model and creating clear link to supporting data we can consider several new relationships that potentially can add significant synergies in respective modelling environment; also defining and implementing metamodel for System Dynamics language would standardise its usage. With System Dynamics tools support those standardization efforts would make possible to have common, searchable model repository, enable interoperability and reuse of models built in different System Dynamics modelling environments.

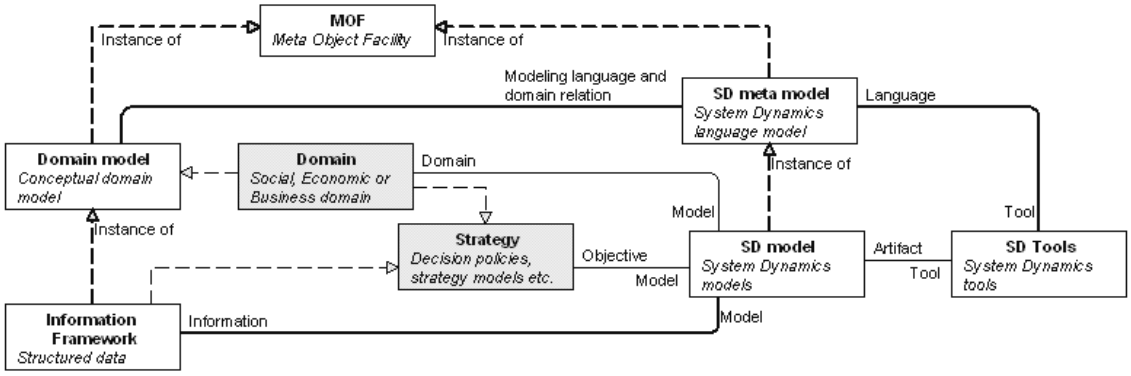

Figure 2. Integrated modelling framework using Meta models

Let's start with domain model. We could say that it formalizes the essence of research domain (e.g. Economic or Social system). It defines the concepts that are used in this domain their attributes and relationships. On top of that concepts can be grouped in packages, sub-systems and in turn their relations can be defined. Analogue to this model in IT industry is often referred to as computation independent model. Model Driven Architecture [6] paradigm is emerging industry wide standard for building information systems and computation independent model is the first and one of the most important models to build. It plays an important role in bridging the gap between those that are experts about the domain and its requirements on the one hand, and those that are experts of the design and construction of the artefacts that together satisfy the domain requirements, on the other. We are not building information system here but we can use the same idea. Even more there are already many successful attempts to create such models in very diverse domains form biology and Gene Expression Specification [7] to Common Information Model built by Electric Power Research Institute [8] that contain common definitions of power system entities and relationships.

Beside that domain model gives significant advantages for data structuring. It adds metadata and allows increment and changing the information in a consistent way. Links to other concepts in the same or related domain can be clearly and unambiguously defined. Model also can serve as a foundation and

reference for further exploration and activities in scientific community. In example considered later in this paper we explore Sustainable Human Development approach. One of the main contributors to approach is United Nations Development Program [9]. The approach is discussed in hundreds if not thousands of different publications, conferences and books. Many other organizations (EU, OECD, several environmental organizations etc.) are dealing with different aspects of sustainable development. Numerous System Dynamics models are built to explore social, economic and environmental feedback loops. Without having common rigorous vocabulary it's very difficult to gain any synergies from those explorations. Again it should be stressed that it is not proposed to have one fully coordinated research program around the world. Nevertheless so long as every researcher who build system dynamic model in certain domain would refer to and use common glossary and would publish their work in structured and standardized way (as proposed in the next chapter) it could bootstrap number of advances. Some of them are described in this paper.

Other important step is structuring the supporting data and adding relationship between domain model and information layer. Advantages that we can get by formalizing this link are twofold. Firstly, whatever measurements or predictions are done for domain instances they can be classified in standardized way. That would also enable much easier search and manipulation of data. System Dynamics modellers would benefit as relevant input and output data would be structured and well defined. Secondly, it would allow sharing and reusing data sets that are driving the model behavior or used to calibrate the model. Acquiring and publishing of input data as well as simulation results could be done in consistent way.

3. System Dynamics Meta model

Why we need to build System Dynamics metamodel and how to use it? System Dynamics metamodel first of all is language syntax definition developed and presented in standardized way e.g. using Meta Object Facility. Built by system dynamics user community metamodel can be used to validate the model syntax and basic semantics. Using well-defined mappings to RDF/XML documents metamodel would define standardized model repository. This would allow storing and retrieving models in the Web and enable model search by its elements or their metadata. If supported by vendors (which is probably the most important practical step) common metamodel would make models tool independent – models build with different tools would be fully compatible.

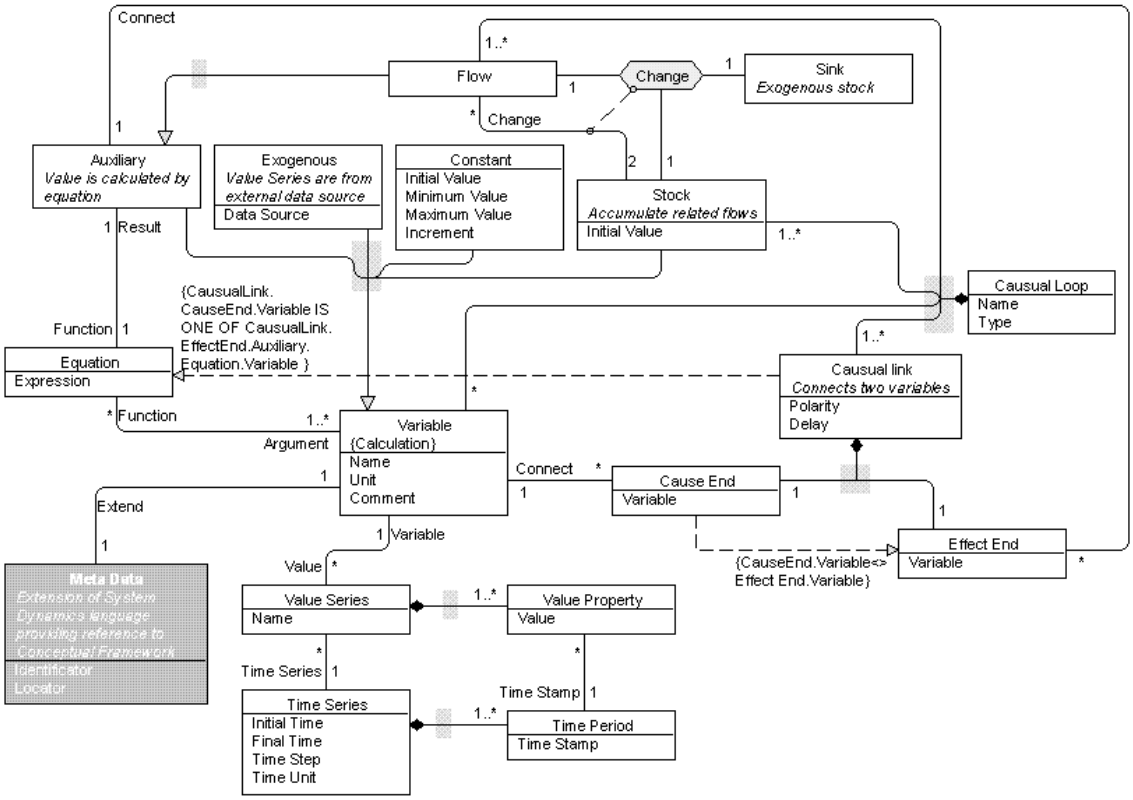

Figure 3. System Dynamics language Meta model

Figure 3 outlines the basic elements of System Dynamics metamodel. Please note that the aim is to illustrate the metamodel concept and it is not intended to build comprehensive System Dynamics metamodel in this paper.

The proposed System Dynamics extension mechanism is marked in grey in Figure 3. The idea here is to add metadata to System Dynamics model elements: stocks, flows, auxiliary, exogenous variables and constants. The extension here is used to define the relation between System Dynamics metamodel and domain model. This relation defines which System Dynamics model elements and by which means can refer to information framework. Thus relationship between language metamodel and domain model structures and formalizes the links between their instances.

4. Modelling sustainable human development approach

As example domain model and information framework for Sustainable Human Development research is sketched in this chapter. Again the aim is to outline the modeling paradigm and not to build full models. There have been some attempts to describe the Sustainable Human Development (SHD) framework in a way that similar to what is discussed in this paper [10]. The difference is that rigorous and well-defined methodology is used here, which is critical to achieve proposed advances.

Sustainable development is conventionally defined as fulfilling "the needs of the present without compromising the ability of future generations to meet their own needs". Many authors have explored theoretical and philosophical foundation of human development. One of the most notable is Nobel prize winner in economics Amartya Sen [11]. His works has inspired also UN development program that has taken the leadership for practical applications in this area. Thus UN Commission on Sustainable Development [12] has defined framework of indicators and methodology to approach SHD. Several states have adopted the approach for their SHD strategies. Figure 4 outlines the main concepts and their relationships of would-be SHD strategy. It is based on UN recommendation and Switzerland experience [13] in building such strategy. Set of themes and postulates are defined in three dimensions - social, economic and environmental. Comprehensive approach in structuring indicators is used. Five indicator stereotypes are defined. References to international agreements and accepted index definitions are explicitly shown. Index value time series are target values are introduced.

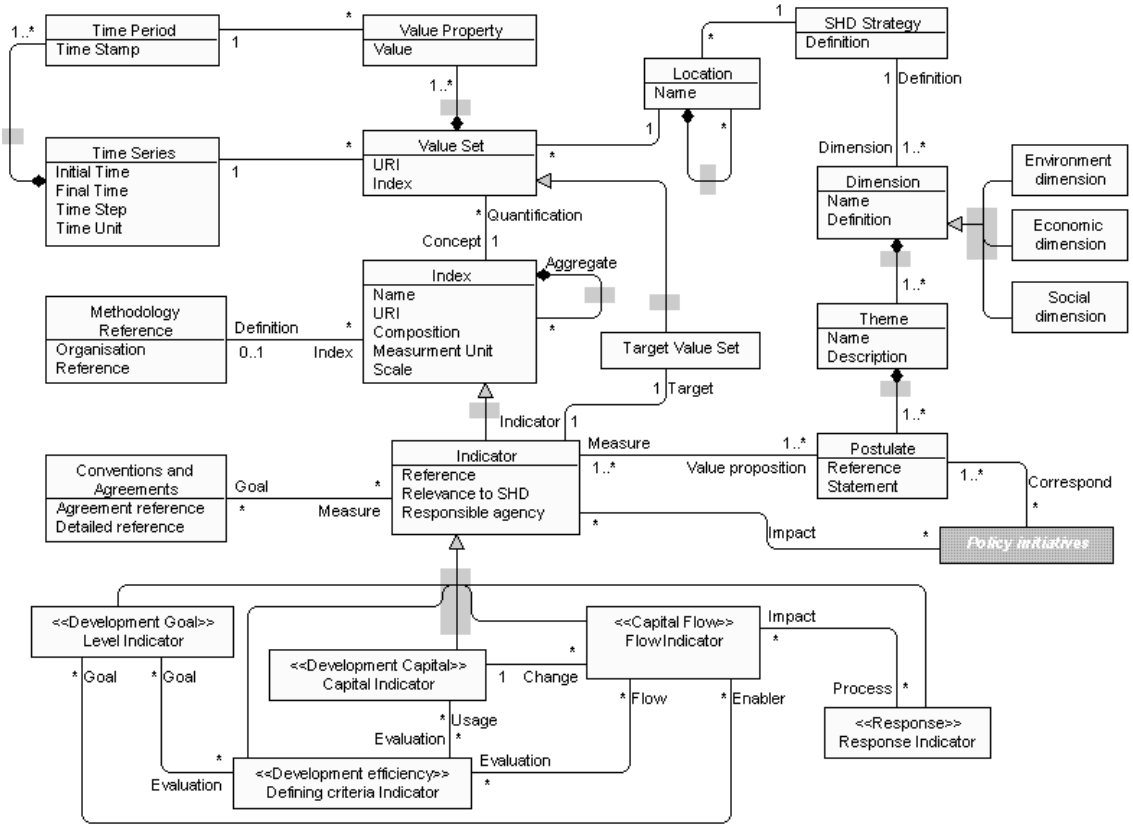

Figure 4. Sustainable human development strategy domain model

It's not intended here to discuss more about SHD approach. Neither is it claimed that domain model that is shown here would be comprehensive or would include all the details. To illustrate the corresponding information the part of the framework is shown on Figure 5.

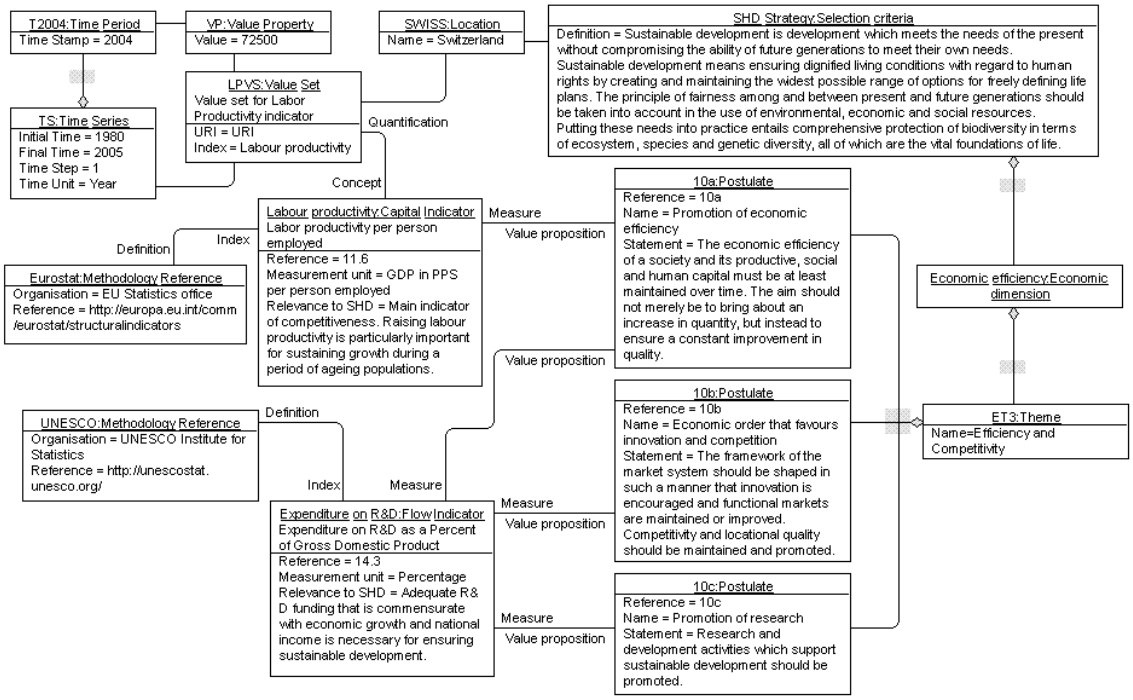

Figure 5. Information framework example

Building the full information framework would be challenging and hopefully rewarding exercise for state or international institutions. However it is shown how the approach can be used to formalize SHD strategy and how those formalizations could enable advances we are aiming for.

To improve understanding how different parts of modelling framework fit together on Figure 6 System Dynamics model with references to information framework are shown.

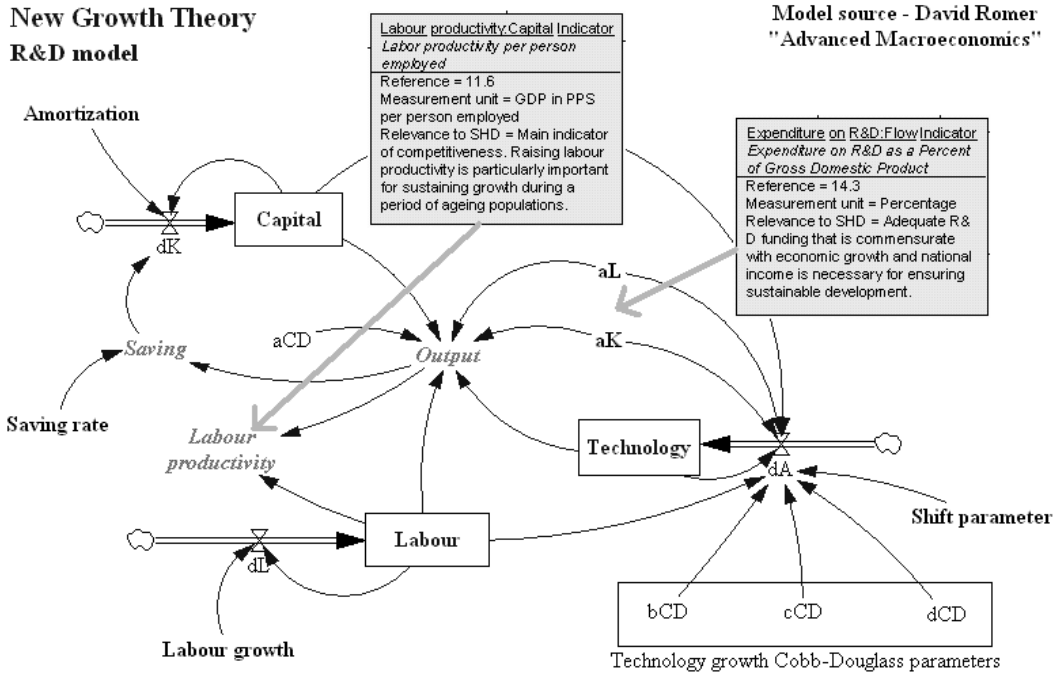

Figure 6. System Dynamics and information framework relation

Here we can explicitly see how System Dynamics model elements could be linked to information framework variables and supporting data. In this case macroeconomic model that describes how investments in research and development impact technology development which in its turn boost the output and labour productivity. In such model number of SHD indicators from information framework example can be calculated. Metadata can be added to those elements and explicit reference to framework indicators can be made.

Thus, if the whole approach would be implemented every modeller that works in certain framework would have straightforward access to the full knowledge base that is accumulated in respective field. For example analyst working in SHD framework that would like to investigate how expenditure on research and development influence labour productivity by simple search in web would be able to retrieve and reuse all the models, supporting data, simulation results and related information that has been created by other analysts around the world.

5. Modelling framework technical implementation

This chapter illustrates how modelling framework could be implemented using standard web technologies. By implementation here I mean transforming the artefacts (System Dynamics models and metamodel, domain model and information framework) in to the form that would enable following advances.

- To have standardised vendor independent repository that can be used to store the artefacts, thus encouraging consistency in manipulating them in all phases of artefact lifecycle.
- To make artefacts available for manipulations with wide range of tool with no loss or corruption of information.
- To make artefacts available in human readable way to the widest possible community (Internet).
- To make artefacts available in machine readable way for search and eventually Semantic Web engines.

The proposed implementation is based on standardized web technologies promoted by World Wide Web Consortium [3]. The Resource Description Framework (RDF) is a language for representing information about resources in the World Wide Web. It is particularly intended for representing metadata about Web resources. RDF is intended for situations in which this information needs to be not only displayed to people but also processed by applications (e.g. search engines) [5]. Models created with MOF can be transformed to RDF documents using well-defined mappings [14]. Relevant parts of domain model and System Dynamics metamodel are transformed to RDF Schema definitions or when technology is matured enough to semantic web ontology's. The most obvious transformation and representation for information framework and System Dynamics models in current state of web technology would be RDF/XML documents.

On Figure 7 the authors give an overview how current independent research activities in Sustainable Human Development could be transformed in to the integrated research framework. The framework implementation using standard Web technologies would allow public and scientific communities collaborating and building common knowledge base and meet the vision introduced in this paper.

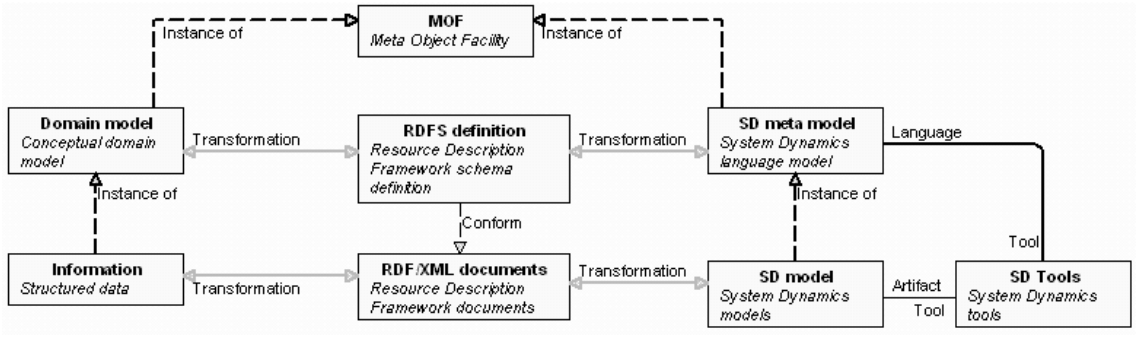

Figure 7. Implementation technical architecture

Summary and conclusions

In the following we will summarize the proposals discussed in this paper. Possible advances arising from them, what needs to be done to reach the results and what could be technical implementation are highlighted.

1. *Building domain model for research domain and formalize information framework.* This activity in many cases might be done quite independently. Indeed OMG [2] has made advances in that area for number of scientific and business domains. In this paper we have highlighted how such models can be built for Sustainable Human Development approach. Formalized domain model and corresponding information can serve as a base for wide range collaboration of researchers working in respective domain. The technical implementation would be based on standardized technologies – class diagram for domain model and information notation and RDF for deployment.

2. *Building and supporting System Dynamics language metamodel.* That would allow standardized use of System Dynamics language, build vendor independent model repositories, exchange and reuse models developed with different tools. If metamodel is build with MOF well defined mappings to RDF could be used for model deployment.

3. *Extending System Dynamics language by adding Meta data to model elements.* This can be used to establish well-defined relationship from System Dynamics model variables to respective research domain model. The most notable advantage from that is possibility to search and reuse models that relate to some part of the research domain. Thus independent modellers could easily facilitate the creation of widely accessible knowledge base. The implementation is done by straightforward extension of System Dynamics metamodel.

4. *Bringing it all out on Web.* The Internet is probably the best media for implementing the proposed framework. That could bootstrap the building and developing integrated but still decentralized scientific knowledge base.

It should be noted that each step that is described here would have its own value and initiatives can be carried out quite independently. Of course the vision cannot be reached without commitment from scientific community, tool vendors and other stakeholders.

References

[1] Sterman John D. (2000) *Business Dynamics*. Irwin/McGraw-Hill.
[2] *Object Management Group*, http://www.omg.org
[3] *World Wide Web Consortium*, http://www.w3.org
[4] *Meta Object Facility Specification*, Version 1.4, Object Management Group.
[5] *Resource Description Framework Primer* (2000) W3C Recommendation / Frank Manola, Eric Miller, eds.
[6] *MDA Guide Version 1.0.1* (2003) Object Management Group.
[7] *Gene Expression Specification, Version 1.1* (2003), October 2003, Object Management Group.
[8] *Electric Power Research Institute*, http://www.epri.com
[9] *Readings in Human Development: Concepts, Measures, and Policies for a Development Paradigm.* (2002) / Edited by Sakiko Fukuda-Parr and A. K. Shiva Kumar.
[10] Grasso Marco, Giulio Enzo Di (2002) *Mapping sustainable development in a capability perspective.* Irwin/McGraw-Hill.
[11] Sen Amartya K. (1999) *Development as freedom.* Anchor Books.
[12] *UN Commission on Sustainable Development,* http://www.un.org/esa/sustdev/csd/csd13/csd13.htm
[13] Altwegg D., Roth I., Scheller A. (2004) *Monitoring Sustainable Development, Final Report: Methods and Results*. Swiss Federal Statistical Office.
[14] Cranefield S. (2001) Networked Knowledge Representation and Exchange using UML and RDF. *Journal of Digital Information* **1**, Issue 8.

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EVALUATION SYSTEM OF RISKY ENTERPRISES

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To differ risky enterprises the special system of evaluation is used now. Revenue office of the Republic of Latvia uses the system named "Eskort". The system must select enterprises that are potentially risky. Such enterprises are first candidates to audit. "Eskort" is a typically additive model of evaluation. The weakness of single level additive model of evaluation is considered in this report. This model is frequently used by test systems and other systems of evaluation. It is very simple but the single level additive model of evaluation cannot realize linear indivisible function. That is why the system for evaluation of risky enterprises cannot solve some problems. Some of them like XOR problem of one level neural network. Multi-layer neural nets and production systems described as the method of overcoming of drawbacks of additive model.

Keywords: *neural nets, evaluation risky enterprises, production system*

1. The weakness of single level additive model of evaluation

A single level additive model of evaluation is frequently used by test systems and other systems of estimation [1]. Essentially the system is one level additive model.

$$T = w_1 x_1 + w_2 x_2 + \ldots w_n x_n, \quad (1)$$

where T is the sum, w_i is the weight of index, x_i is the index, n is the quantity of indexes. The principal weakness follows from additive evaluation. Consider examples.

Example 1.
If the enterprise has one employee and high turnover then it is a "risky" enterprise. If the kind of enterprise activity is a "middleman" then the enterprise is not "risky" (such combination of characteristics is acceptable).

Example 2.
If we have a new enterprise then it is necessary to increase all indexes value (new enterprises are the most risky enterprises).
From examples follows that we must evaluate from combination parameters or we must correct index value during evaluation. Obviously, we cannot do that by means of changing values of indexes. Thus we can solve these tasks by using neural nets and production systems.

TABLE 1. Risky Indexes

Mark	Index	Value
x1	employee	1, if 1 employee, 0 otherwise
x2	turnover	1, if «big», 0 otherwise
x3	kind of activity	1, if «middleman» , 0 otherwise

We will use a pad-neuron [2]. Mathematical model of a pad-neuron is $y = f\left(\frac{\sum_{i=1} a_i x_i + a_0}{\sum_{i=1}^{n} b_i x_i + b_0}\right)$.

Where f is the threshold function of activity

$$f(g)=\begin{cases}"risk", g<1\\ "normal", g\geq 1\end{cases},$$

[if $a0=b0=0$, $a1=a2=a3=1$ and $b1=b2=1$, $b3=2$, $x3=0$, $x2=x1=1$ then f (g) > 1,
else $x3=x2=x1=1$, then $f(g)<1$].

It is significant that threshold function is equivalent of rule: if $g<1$ then "*risk*" else "*normal*".

Therefore we can use production system (1=*True* and 0=*False*) also to solve tasks. We can use two rules only.

Example 3
Rule 1: IF x1 AND x2 AND x3 THEN "*normal*".

Example 4
Rule 2: IF x4 THEN "increase weight of all indexes".
Let us suppose that production system is equivalent of neural. That is not true. Consider next example.

Example 5. Training system.
Suppose that the system work well if the student can answer only one question from two.

Q1 \ Q2	1	0
1	B	A
0	A	B

Q1, Q2 are questions. A, B are conclusion. A – the effective training system, B – otherwise.

Example 5. Enterprises.

T \ E	1	0
1	A	B
0	B	A

T – turnover (1 – low, 0 – high), E – employees (1 – many, 0 – single). Suppose that A is a risky enterprise, B – otherwise. We cannot differ A and B by changing weight of a pad-neuron. However, a new rule *IF* $Q_1 = Q_2$ *THEN A ELSE B* easy solves the task.

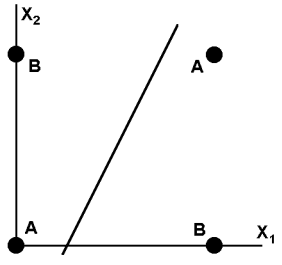

Figure 1. Types of business situations

The principal weakness of present system is the same as the well-known XOR problem in one level neural net. The model (1) is the model of hyper plane in n-dimensional space. It is line in a 2-dimensional space. The line (hyper plane) cannot divide some types of situations (Figure 1).

So, the single level additive model of evaluation cannot realize linear indivisible function. We can solve the situation like it is showed on Fig. 1 by using multi-layer evaluation system. For example, two layer neural network:

$$T = f_2\left(\sum_{i=1}^{N} w_{2i}\, f_1\left(\sum_{k=1}^{K} w_{1k}\, x_k\right)\right).$$

2. Evaluation system of risky enterprises

Revenue office of the Republic of Latvia uses the system named "Eskort" for an evaluation of risky enterprises [3]. Main task of the system is choosing of enterprises for audit. The system selects enterprises by using special indexes and penalty marks. It evaluates indexes by using a system of rules and calculates the sum. As result the enterprise with a maximal sum becomes the first candidate to be audited (Figure 2).

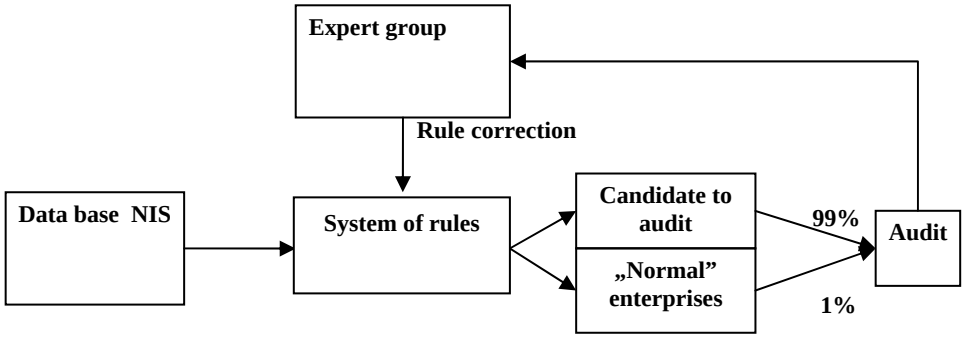

Figure 2. Evaluation system's functioning

3. The weakness of the present system and ways of improvement

The present system has same drawbacks. First of them is an additive evaluation of risk. The second drawback is the manual correction of rules. Thus, we can overcome this weakness by using of multi-layer neural nets and production systems. Both ways have advantages and disadvantages. A production system with a direct line of reasoning is considered. The system may be created if experts can formulate all rules of evaluation. Moreover, the production system can work if rules are stable. The application of multi-layer neural nets is more appropriate if experts cannot formulate rules and\or rules are not stable. In this case, we can teach net in the process of use. We propose the adaptive system of evaluation of the risk of enterprises (Figure 3).

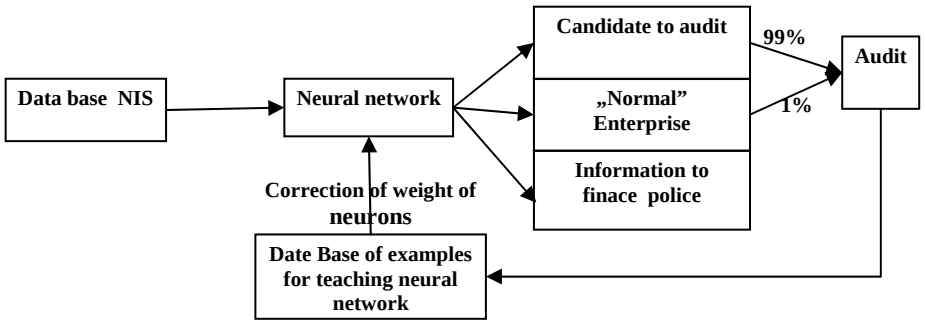

Figure 3. The adaptive system of the evaluation of risky enterprises

Conclusion

The single level additive model of an evaluation cannot realize the linear indivisible function. Thus, we can overcome this weakness by using multi-layer neural nets and production systems. Production system may be created if experts can formulate all rules of evaluation. Moreover, the production system can work if rules are stable. The application of multi-layer neural nets is more appropriate if experts cannot formulate rules and\or rules are not stable. In this case, we can teach net in the process of use. So, we can propose the adaptive evaluation system of risky enterprises.

Acknowledgment

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References

[1] Anastazi A., Urbina S. (2003) *Psychological testing.* St.Petersburg: Piter.
[2] *Neirocomputers* (2002) Moscow: Bauman MSTU. 320 p.
[3] Nodokļu kontroles process, http://www.vid.gov.lv/default.aspx?tabid=8&id=1005&hl=1[NL][NL]

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NEW STATISTICAL CHARACTERISTICS FOR MINING FREQUENT SEQUENCES IN LARGE DATABASES

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The paper deals with the search and analysis of the subsequence in large volume sequences (texts, DNA sequences, etc.). A new algorithm ProMFS for mining frequent sequences is proposed and investigated. It is based on the estimated probabilistic-statistical characteristics of the appearance of elements of the sequence and their order. The algorithm builds a new much shorter sequence and makes decisions on the main sequence in accordance with the results of analysis of the shorter one.

Keywords: *Data Mining, frequent sequences*

1. Introduction

Generally, data mining (sometimes called data or knowledge discovery) is the process of analysing data from different perspectives and summarizing it into useful information – information that can be used to increase revenue, cuts costs, or both. Data mining software is one of a number of analytical tools for analysing data. It allows users to analyse data from many different dimensions or angles, categorize it, and summarize the relationships identified. Technically, data mining is the process of finding correlations or patterns among dozens of fields in large relational databases.

Although data mining is a relatively new term, the technology is not. Companies have used powerful computers to sift through volumes of supermarket scanner data and analyse market research reports for years. However, continuous innovations in computer processing power, disk storage, and statistical software are dramatically increasing the accuracy of analysis while driving down the cost.

Data are any facts, numbers, or text that can be processed by a computer. Today, organizations are accumulating vast and growing amounts of data in different formats and different databases. This includes:

1) operational or transactional data such as, sales, cost, inventory, payroll, and accounting;
2) non-operational data;
3) meta data.

The patterns, associations, or relationships among all this *data* can provide *information*. Information can be converted into *knowledge* about historical patterns and future trends.

Dramatic advances in data capture, processing power, data transmission and storage capabilities are enabling organizations to integrate their various databases into *data warehouses*. Data warehousing is defined as a process of centralized data management and retrieval. Data warehousing, like data mining, is a relatively new term although the concept itself has been around for years. Data warehousing represents an ideal vision of maintaining a central repository of all organizational data. Centralization of data is needed to maximize user access and analysis. Dramatic technological advances are making this vision a reality for many companies. And, equally dramatic advances in data analysis software are allowing users to access this data freely. The data analysis software is what supports data mining.

Companies primarily use data mining today with a strong consumer focus such as retail, financial, communication and marketing organizations. It enables these companies to determine relationships among "internal" factors such as price, product positioning or staff skills, and "external" factors such as economic indicators, competition, and customer demographics. Moreover, it enables them to determine the impact on sales, customer satisfaction and corporate profits. Finally, it enables them to "drill down" into summary information to view detail transactional data.

Data mining consists of five major stages:
1. Extract, transform and load transaction the data onto the data warehouse system.
2. Store and manage the data in a multidimensional database system.
3. Provide data access to business analysts and information technology professionals.
4. Analyse the data by application software.
5. Present the data in a useful format, such as a graph or table.

Different levels of analysis are available:
1. Artificial neural networks;
2. Genetic algorithms;
3. Decision trees;
4. Nearest neighbour method;
5. Rule induction;
6. Data visualization.

2. Sequential pattern mining

Sequential pattern mining [3-6], which finds the set of frequent subsequence in sequence databases, is an important data mining task and has broad applications, such as business analysis, web mining, security and bio-sequences analysis. We will examine just plain text information. Text mining is a variation of a field called data mining that tries to find interesting patterns from large databases. The difference between regular data mining and text mining is that in text mining the patterns are extracted from natural language text rather than from structured databases of facts. Databases are designed for programs to process automatically; a text is written for people to read. Text mining methods can be used in bio-informatics for analysis of DNA sequences. A DNA sequence (sometimes genetic sequence) is a succession of letters representing the primary structure of a real or hypothetical DNA molecule or strand. The possible of sequence letters are A, C, G, and T, representing the four nucleotide subunits of a DNA strand (adenine, cytosine, guanine, thymine), and typically these are printed abutting one another without gaps, as in the sequence AAAGTCTGAC (see [2] for details).

The problem of mining sequential patterns is formulated, e.g., in [3, 4]. Assume we have a set $L=\{i_1, i_2, \ldots, i_m\}$ consisting of m distinct elements, also called *items*. An *item set* is a nonempty unordered collection of items. A *sequence* is an ordered list of item-sets. A *sequence* α is denoted as $(\alpha_1 \rightarrow \alpha_2 \rightarrow \ldots \rightarrow \alpha_q)$, where the sequence *element* α_j is an *item set*. An item can occur only once in an item set, but it can occur multiple times in different item sets of a sequence [4]. We solve a partial problem, where *item set* consists of one item only. A sequence $\alpha=(\alpha_1 \rightarrow \alpha_2 \rightarrow \ldots \rightarrow \alpha_n)$ is a *subsequence* of another sequence $\beta=(\beta_1 \rightarrow \beta_2 \rightarrow \ldots \rightarrow \beta_m)$, if there exist such numbers $t_1, t_2, \ldots, t_n$, where $t_{j+1} = t_j + 1,\ j = 1, \ldots, n$ and $\alpha_j = \beta_{t_j}$ for all a_j. Here β_{t_j} are elements of the set L. We analyse a sequence (the main sequence) S that is formed from single elements of L (not their sets, as is used in the classical formulation [3, 4] of the problem). In general, the number of elements in S is much larger than that in L. We have to find the most frequent subsequence in S. The problem is to find subsequence whose appearance frequency is more than some threshold called minimum support, i.e. the subsequence is frequent if it occurs in the main sequence not less than the minimum support times.

The most popular algorithm for mining frequent sequences is the GSP (Generated Sequence Pattern) algorithm. It has been examined in a lot of publications (see, e. g., [1, 3]). While searching frequent sequences in a long text, a multiple reviewing is required. The GSP algorithm minimizes the number of reviewing, but the searching time is not satisfactory for large sequence volumes. Other popular algorithms are. SPADE [3], PrefixSpan [8], FreeSpan [9] and SPAM [10].

In this paper, a new algorithm for mining frequent sequences (ProMFS) is proposed. It is based on estimated statistical characteristics of the appearance of elements of the main sequence and their order. It is an approximate method. The other method of this class is ApproxMAP [11]. The general idea of ApproxMAP is that, instead of finding exact patterns, it identifies patterns approximately shared by many sequences. The difference of our method is that we estimate the probabilistic-statistical characteristics of elements of the sequence database, generate a new much shorter sequence and make decisions on the main sequence in accordance with the results of analysis of the shorter one.

3. GSP (Generated Sequence Pattern) algorithm

Let us note that if the sequence is frequent, each its possible subsequence is also frequent. For example, if the sequence *AABA* is frequent, all its subsequence *A*, *B*, *AA*, *AB*, *BA*, *AAB*, and *ABA* are

frequent, too. Using this fact, we can draw a conclusion: if a sequence has at least one infrequent subsequence, the sequence is infrequent. Obviously, if a sequence is infrequent, all newly generated (on the second level) sequences will be infrequent, too.

At first we check the first level sequences. We have m sequences. After defining their frequencies, we start considering the second level sequences. There will be m^2 of such sequences (i_1i_1, i_1i_2, ..., i_1i_m, i_2i_1, ..., i_2i_m, ..., i_mi_1, ..., i_mi_m). However, we will not check the whole set of sequences. According to the previous level, we will only define which sequences should be checked and which not. If the second level sequence includes an infrequent sequence of the previous level (first level), then it is infrequent and we can eliminate it even without checking it up. Let us analyse an example. Suppose that some sequence is given:

$S = ABCCCBBCABCABCABCBABCCCABCAABABCABC.$ (1)

We will say that the sequence is frequent if it occurs in the text not less than 4 times, i.e. the minimum support is equal to 4. Frequent sequences will be A, B, C, AB, BC, CA, CC, ABC, BCA, CAB.

4. The probabilistic algorithm for mining frequent sequences (ProMFS)

The new algorithm for mining frequent sequences is based on the estimation of the statistical characteristics of the main sequence:

- the probability of an element in the sequence,
- the probability for one element to appear after another one,
- the average distance between different elements of the sequence.

The main idea of the algorithm is following:

1) some characteristics of the position and interposition of elements are determined in the main sequence;
2) a new much shorter model sequence $\widetilde{C}$ is generated according to these characteristics;
3) a new sequence is analysed with the GSP algorithm (or any similar one);
4) the subsequence frequency in the main sequence is estimated by the results of the GSP algorithm applied on the new sequence.

Let:

1) $P(i_j) = \dfrac{V(i_j)}{VS}$ be the probability of occurrence of element i_j in the main sequence, where $i_j \in L,\ j = 1,...,m$. Here $L=\{i_1, i_2, \ldots, i_m\}$ is the set consisting of m distinct elements. $V(i_j)$ is the number of elements i_j in the main sequence S; VS is the length of the sequence. Note that $\sum_{j=1}^{m} P(i_j) = 1$.

2) $P(i_j \mid i_v)$ be the probability of appearance of element i_v after element i_j, where $i_j, i_v \in L,\ j, v = 1,...,m$. Note that $\sum_{v=1}^{m} P(i_j \mid i_v) = 1$ for all $j = 1,...,m$.

3) $D(i_j \mid i_v)$ be the distance between elements i_j and i_v, where $i_j, i_v \in L,\ j, v = 1,...,m$. In other words, the distance $D(i_j \mid i_v)$ is the number of elements that are between i_j and the first found i_v seeking from i_j to the end of the main sequence, where $D(i_j \mid i_v)$ includes i_v. The distance between two neighbouring elements of the sequence is equal to one.

4) $\widehat{A}$ be the matrix of average distances. Elements of the matrix are as follows: $a_{jv} = Average\ (D(i_j \mid i_v),\ i_j, i_v \in L),\ j, v = 1,..., m.$ All these characteristics can be obtained during one search through the main sequence. According to these characteristics a much shorter model sequence $\widetilde{C}$ is generated. The length of this sequence is l. Denote its elements by c_r, $r = 1,...,l$. The model sequence $\widetilde{C}$ will contain elements from L: $i_j \in L,\ j = 1,...,m$. For the elements c_r, a numeric characteristic $Q(i_j, c_r)$, $r = 1,...,l$, $j = 1,...,m$, is defined. Initially, $Q(i_j, c_r)$ is the matrix with zero values that are specified after the statistical analysis of the main sequence. A complementary function $\rho(c_r, a_{rj})$ is introduced. This function increases the value of characteristics $Q(i_j, c_r)$ by one. The first element c_1 of

the model sequence $\widetilde{C}$ is that from *L*, that corresponds to $\max(P(i_j))$, $i_j \in L$. According to c_1, it is activated the function $\rho(c_1, a_{1j}) \Rightarrow Q(i_j, 1+a_{1j}) = Q(i_j, 1+a_{1j}) + 1$, $j = 1,...,m$. Remaining elements c_r, $r = 2,...,l$, are chosen in the way below. Consider the *r*-th element c_r of the model sequence $\widetilde{C}$. The decision, which symbol from *L* should be chosen as c_r, will be made after calculating $\max(Q(i_j, c_r))$, $i_j \in L$. If for some *p* and *t* we obtain that $Q(i_p, c_r) = Q(i_t, c_r)$, then element c_r is chosen by maximal value of conditional probabilities, i.e. by $\max(P(c_{(r-1)} \mid i_p), P(c_{(r-1)} \mid i_t))$: $c_r = i_p$ if $P(c_{(r-1)} \mid i_p) > P(c_{(r-1)} \mid i_t)$, and $c_r = i_t$ if $P(c_{(r-1)} \mid i_p) < P(c_{(r-1)} \mid i_t)$. If these values are equal, i.e. $P(c_{(r-1)} \mid i_p) = P(c_{(r-1)} \mid i_t)$, then c_r is chosen in dependence on $\max(P(i_p), P(\mid i_t))$. After choosing the value of c_r, the function $\rho(c_r, a_{rj}) \Rightarrow Q(i_j, r+a_{rj}) = Q(i_j, r+a_{rj}) + 1$ is activated. All these actions are performed consecutively for every $r = 2,...,l$. In such way we get the model sequence $\widetilde{C}$, which is much shorter than the main one and which may be analysed by the GSP algorithm with much less computational efforts.

Consider the previous example with the main sequence (1) given in Section 2. *L*={*A, B, C*}, i.e. *m*=3, $i_1 = A$, $i_2 = B$, $i_3 = C$. The sequence has *VS*=35 elements.

After one checking of this sequence such probabilistic characteristic are calculated:

$$P(A) = \frac{10}{35} \approx 0.2857,\ P(B) = \frac{12}{35} \approx 0.3429,\ P(C) = \frac{13}{35} \approx 0.3714,\ P(A \mid A) = 0.1,$$

$$P(A \mid B) = 0.9,\ P(A \mid C) = 0,\ P(B \mid A) \approx 0.1667,\ P(B \mid B) = 0.0833,$$

$$P(B \mid C) \approx 0.7500,\ P(C \mid A) \approx 0.4615,\ P(C \mid B) = 0.1538,\ P(C \mid C) \approx 0.3077.$$

TABLE 1. The matrix $\widehat{A}$ of average distances

	A	*B*	*C*
A	3.58	1.10	2.50
B	2.64	2.91	1.42
C	2.33	2.25	2.67

Let us compose a model sequence $\widetilde{C}$, whose length is *l*=8. At the beginning, the sequence $\widetilde{C}$ is empty, and $Q(i_j, c_r) = 0$, $r = 1,...,l$, $j = 1,...,m$:

r	1	2	3	4	5	6	7	8
A	0	0	0	0	0	0	0	0
B	0	0	0	0	0	0	0	0
C	0	0	0	0	0	0	0	0
Model sequence $\widetilde{C}$	-	-	-	-	-	-	-	-

The first element of $\widetilde{C}$ is determined according to the largest probability $P(i_j)$. In our example, it is *C*, i.e. $c_1 = C$. Recalculate $Q(i_j, c_1)$, $j = 1,2,3$, according to the average distances. The situation becomes as follows:

r	1	2	3	4	5	6	7	8
A	0	0	**1**	0	0	0	0	0
B	0	0	**1**	0	0	0	0	0
C	0	0	0	**1**	0	0	0	0
Model sequence $\widetilde{C}$	***C***							

Let us choose c_2. All three values $Q(i_j, c_1)$, $j = 1,2,3$, are equal. Moreover, they are equal to zero; therefore, c_2 will be determined by maximal value of conditional probabilities. max(*P*(*C*|*A*), *P*(*C*|*B*), *P*(*C*|*C*)=*P*(*C*|*A*)= 0.4615. Therefore, $c_2 = A$. Recalculate $Q(i_j, c_2)$, $j = 1,2,3$, according to the average distances. The situation becomes as follows:

r	1	2	3	4	5	6	7	8
A	0	0	1	0	0	**1**	0	0
B	0	0	**2**	0	0	0	0	0
C	0	0	0	1	**1**	0	0	0
Model sequence $\widetilde{C}$	*C*	***A***						

Next three steps of forming the model sequence are given below:

r	1	2	3	4	5	6	7	8
A	0	0	1	0	0	**2**	0	0
B	0	0	2	0	0	1	0	0
C	0	0	0	**1**	**2**	0	0	0
Model sequence $\widetilde{C}$	*C*	*A*	***B***					

r	1	2	3	4	5	6	7	8
A	0	0	1	0	0	**3**	0	0
B	0	0	2	0	0	**2**	0	0
C	0	0	0	1	2	0	**1**	0
Model sequence $\widetilde{C}$	*C*	*A*	*B*	***C***				

r	1	2	3	4	5	6	**7**	8
A	0	0	1	0	0	3	**1**	0
B	0	0	2	0	0	2	**1**	0
C	0	0	0	1	2	0	1	**1**
Model sequence $\widetilde{C}$	*C*	*A*	*B*	*C*	***C***			

The resulting model sequence is $\widetilde{C} = CABCCABC$. The GSP algorithm has determined that the longest frequent subsequence of the model sequence is *ABC* when the minimum support is set to 2. Moreover, the GSP algorithm has determined the second frequent subsequence *CAB* of the model sequence for the same minimum support. In the main sequence (1), the frequency of *ABC* is 8 and that of *CAB* is 5. However, the subsequence *BCA*, which frequency is 5, has not been determined by the analysis of the model sequence. One of the reasons may be that the model sequence is too short.

5. Experimental results

The probabilistic mining of frequent sequences was compared with the GSP algorithm. We have generated the text file of 100000 letters (1000 lines and 100 symbols in one line). $L=\{A, B, C\}$, i.e. $m = 3$, $i_1 = A$, $i_2 = B$, $i_3 = C$. In this text we have included one very frequent sequence *ABBC*. This sequence is repeated 20 times in one line. The remaining 20 symbols of the line are selected at random. First of all, the main sequence (100000 symbols) was investigated with the GSP algorithm. The results are presented in Figures 1 and 2. They will be discussed more in detail together with the results of ProMFS. ProMFS generated the following model sequence $\widetilde{C}$ of length $l = 40$:

$\widetilde{C} = BBCABBCABBCABBCABBCABBCABBCABBCABBCABBCA.$

This model sequence was examined with the GSP algorithm using the following minimum support: 8, 9, 10, 11, 12, 13 and 14. The results are presented in Figures 1 and 2. Fig. 1 shows the number of frequent sequences found both by GSP and ProMFS. Fig. 2 illustrates the consumption of computing time used both by GSP and ProMFS to obtain the results of Figure 1 (the minimum support in ProMFS is *Ms*=8; the results are similar for larger *Ms*). The results in Figure 1 indicate that, if the minimum support in GSP analysing the main sequence is comparatively small (less than 1500 with the examined data set), GSP finds much more frequent sequences than ProMFS. When the minimum support in GSP grows from 2500 till 6000, the number of frequent sequences by GSP decreases and by ProMFS increases. In the range of [2500, 6000], the number of frequent sequences found both by GSP and ProMFS is rather similar. When the minimum support in GSP continues growing, the number of frequent sequences found by both algorithms becomes identical. When comparing the computing time of both algorithms (see Figure 2), we can conclude that the ProMFS operates much faster. In the range of the minimum support in GSP [2500, 6000], ProMFS needs approximately 20 times less of computing time as compared with GSP to obtain the similar result.

Conclusions

The new algorithm ProMFS for mining frequent sequences is proposed. It is based on the estimated probabilistic-statistical characteristics of the appearance of elements of the sequence and their order: the probability of an element in the sequence, the probability for one element to appear after another one, and the average distance between different elements of the sequence. The algorithm builds a new, much shorter model sequence, and makes decision on the main sequence in accordance with the results of analysis of the shorter one. The model sequence may be analysed by the GSP or other algorithm for mining frequent sequences: the subsequence frequency in the main sequence is estimated by the results of the model sequence analysis. The experimental investigation indicates that the new algorithm allows saving the computing time in a large extent. It is very important when analysing very large data sequences.

Moreover, the model sequence, that is much shorter than the main one, may be more understandable and easily perceived: in the experimental investigation, the sequence of 100000 elements has been modelled by a sequence of 40 elements. However, the sufficient relation between the length of the model sequence and the main sequence needs a more thorough investigation – both theoretical and experimental. In the paper, we present the experimental analysis of the proposed algorithm on the artificial data only. Further research should prove the efficiency on the real data. The research should disclose the optimal values of algorithm parameters (e.g. the length l of the model sequence $\widetilde{C}$, the minimum support for analysis of the model sequence). Another perspective research direction is the development of additional probabilistic-statistical characteristics of large sequences. This may produce the model sequence that is more adequate to the main sequence.

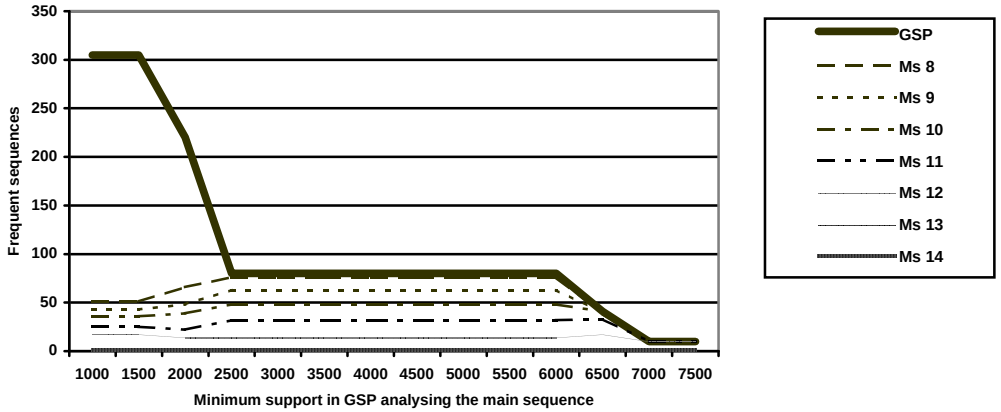

Figure 1. Number of frequent sequences found both by GSP and ProMFS (minimum support in ProMFS is *Ms* = 8,…,14)

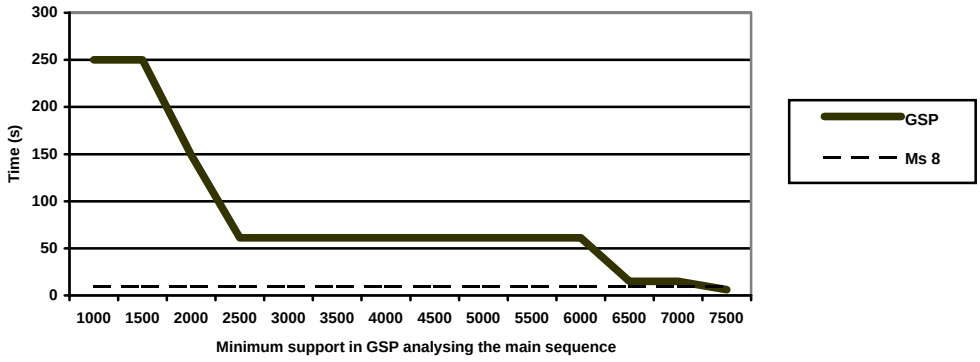

Figure 2. Computing time used both by GSP and ProMFS (minimum support in ProMFS is *Ms* = 8)

References

[1] Agrawal R. C., Agrawal C. C., Prasad V. V. (2000) Depth first generation of long patterns. In: *Proceedings of the Sixth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. Boston, Massachusetts, 108-118.

[2] http://en.wikipedia.org/wiki/DNA_sequence

[3] Zaki M. J. (2001) SPADE: An efficient algorithm for mining frequent sequences. *Machine Learning Journal* **42** (1/2), 31-60. (D. Fisher, ed. Special issue on Unsupervised Learning)

[4] Zaki M.J. (2000) *Parallel sequence mining on shared-memory machines. In: Large-scale Parallel Data Mining. Lecture Notes in Artificial Intelligence* / M. J. Zaki, Ching-Tien Ho, eds. Vol. 1759. Berlin, Heidelberg, New York: Springer-Verlag, 161-189.

[5] Pei P. J., Han J., Wang W. (2002) Mining Sequential Patterns with Constraints in Large Databases. In: *Proceedings of the 11th ACM International Conference on Information and Knowledge Management (CIKM'02)*. McLean, VA, 18-25.

[6] Pinto P., Han J., Pei J., Wang K., Chen Q., Dayal U. (2001) Multi-Dimensional Sequential Pattern Mining. In: *Proceedings of the 10th ACM International Conference on Information and Knowledge Management (CIKM'01)*. Atlanta, Georgia, 81-88.

[7] Pei J., Han J., Mortazavi-Asl B., Pinto H., Chen Q., Dayal U., Hsu M.-C. (2001) PrefixSpan: Mining sequential patterns efficiently by prefix-projected pattern growth. In: *Proc. 17th International Conference on Data Engineering ICDE.* Heidelberg, 215-224.

[8] Han J., Pei J. (2000) FreeSpan: Frequent pattern-projected sequential pattern mining. In*: Proc. Knowledge Discovery and Data Mining.* 355-359.

[9] Ayres J., Flannick. J., Gehrke J., Yiu T. (2002) Sequential pattern mining using a bitmap representation. In*: Proc. Knowledge Discovery and Data Mining.* 429-435.

[10] Kum H. C., Pei J., Wang W. (2003) ApproxMAP: Approximate Mining of Consensus Sequential Patterns. In: *Proceedings of the 2003 SIAM International Conference on Data Mining (SIAM DM '03)*. San Francisco, CA, 311-315.

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THE ECONOMETRIC MODELS OF FORECASTING OF THE TRANSPORT FLOWS

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The importance of forecasting the economic characteristics of transportation (i.e. the amount of freight and passengers carried, the turnover rate of freight and passengers, etc. in transportation as a whole and in particular areas using various transport facilities) is demonstrated. Methods for predicting the development of transportation based on multidimensional regression and correlation analysis and realizing mathematical models for finding linear and non-linear multidimensional regression equations as well as a mathematical model for choosing linear and non-linear regression equations, more accurately approximating the empirical data, are presented.

The techniques aimed to obtain and apply the linear correlation coefficient and correlative relationship in determining the forecast accuracy is also given. The efficiency of methods, determining the linear correlation coefficient and correlative relationship, used in achieving higher accuracy of forecasts is shown.

Keywords: *forecasting, multidimensional regression, correlative analysis, mathematical models, approximation, empirical data, correlative relationship, linear correlation coefficient*

1. Introduction

National Transportation Development Programme, compiled in 1993 and approved by the Lithuanian Government in 1994, embraces the period up to 2010. It has played an important role in the reconstruction and development of the Lithuanian transport system. This programme has also been approved by other countries. However, European and other countries usually revise their transport strategies every four or five years. The same need is found in the Republic of Lithuania. A number of objective factors exist conditioning the necessity to make corrections in the National Transport Development Programme. Primarily, the policy of our country is to integrate into the EC as well as to follow new trends of transport development both in Europe and other countries (i.e. multimodal transport development, increasing requirements of transport to ensure environmental protection, the growth of the transportation services market, etc.).

Two out of 17 units of the National Transport Development Programme concern the forecasting of transport infrastructure development. They are as follows:

1. Current situation in the transport sector and its development trends;
2. The development of road, railroad, water and air transport (when integrating into the EC transport network).

This makes it necessary to compile one of the most important sections of a new development programme associated with the description of the present state of all means of transport and their development trends. The latter should include the forecasts for transporting freight and passengers by road, railroad, water and air transport in 2005, 2010 and 2015.

To predict this the application of two-dimensional regression and correlation analyses [1] is not sufficient. In this case transport development should be considered in the context of the development of the national economy, and transport as its particular branch. The major factors as well as their interrelation and effect on the development of this or that means of transport should be evaluated. General indices characterising the economic state of the country may be considered gross output, national income, volume of output, etc. Therefore, the selection of suitable regression equations to predict the economic characteristics of transport (i.e. the volume of freight and passengers' transit, freight and passengers' turnover, etc. with respect to both transport system and its particular branch) requires the application of multidimensional regression and correlation analyses [2–5].

2. The reliability of forecasts in transportation

Forecasting transportation is one of the major goals of a multistage complex program of transport development in Lithuania. It is one the most complicated problems, however, too little attention is being

paid to it in specialist literature. Unlike the problem of planning, it has only been analysed by a few researchers. Therefore, in the present paper, emphasis is placed on the urgent transport problems associated with making forecasts and the reliability of these forecasts.

The problem of forecasting may be formulated as follows: let $Y = \{y(t_i)\}$ be a one-dimensional time series of statistical observations $t_{i+1} - t_i = \text{const}$ in the particular time moments, where $i = 1, ..., n$. The problem is to find the moments t_j, where $j = n+1, ..., n+T$. Moreover, the inertia of the investigated process is assumed as maintaining a general trend in time.

The level of the time series at the moment t may be determined by summing up two components:

$$y = f(\Theta, t) + \varepsilon(t), \tag{1}$$

where $f(\Theta, t)$ is a certain constant time function (trend); $\varepsilon(t)$ is a function assessing the effect of stochastic factors (agents); Θ is the parameter vector to be determined.

In formula (1), $f(\Theta, t)$ describes the main trends of the process analysed, assessing the effects of major factors on this process. This implies that if $f(\Theta, t)$, a constant component of the process, could be determined; then $\varepsilon(t)$ – the remaining component – would be random, thus proving that the process is stochastic.

In order to determine $f(\Theta, t)$, the regression and correlation analysis is applied.

Normally, a researcher analyses a certain phenomenon, quantitatively describing the value y, which varies because of certain factors, which in turn are quantitatively determined by the values, which the researcher deliberately changes to cause the variation of the analysed value y.

Let us suppose that the particular value y_1 of the analysed value y corresponds to the particular set of values $(x_1, z_1, ..., t_1)$ of the variables $x, z, ..., t$; while the value y_2 corresponds to another set $(x_2, z_2, ..., t_2)$, etc. It means that there is a certain relationship between the variables $x, z, ..., t$ and the analysed value y. It may be a functional relationship or correlation.

Correlation analysis allows us to determine the extent of the dependence of the value y on the variables $x, z, ..., t$. Based on correlation as well as linear and non-linear correlation analysis, it is possible to determine which of the factors characterised by the values $x, z, ..., t$, are relevant, which have only a small effect on the value y, and which are completely irrelevant to this value. Clearly observed correlations allow us to make an assumption that, in this case, not only correlations but functional relationships might be found as well. The latter may be described by the regression equations. Having obtained an analytical expression $y = f(x, z, ..., t)$ for a functional relationship between a set $(x, z, ..., t)$ and the analysed value y in this way, it can be extrapolated, i.e. y values, related to the values of the variables $x, z, ..., t$, lying outside the interval of values used in the tests, may be determined. Extrapolation is the basis of forecasting made for the particular phenomena under varying conditions.

The analytical expression of a functional relationship based on regression analysis may be sought if the type of function could be established first. If this is not feasible, the relationship may be simulated, based on the principle of simplicity of a mathematical model. Such problems make the basis for the application of mathematical simulation techniques involving the approximation of functional relationship by polynomials and the probability approach.

3. The establishment of linear and non-linear correlation between four variables of the regression equation

The application of multidimensional regression and correlation analysis for a simple case of establishing the relationship between three variables has been described [1].

However, a comparative analysis of the forecasts and statistical data revealed that the above forecasts obtained by non-linear three variables or second-order regression equations were not always reliable [2–7].

If a relationship exists between t, x, z and y, for example, t – time periods, x – gross national product, z – volume of production or national income, with y being freight (passengers) turnover, then, when the relationship is linear, we obtain:

$$y' = at + bx + cz + d \tag{2}$$

while in case of a non-linear (second-order) relationship, we obtain:

$$y'' = at^2 + bt + cx^2 + dx + ez^2 + fz + g\ . \tag{3}$$

The problem is to calculate the parameters a, b, c and d of the regression equations (2), and the parameters a, b, c, d, e, f and g of (3). This problem can be solved in a similar way to that which was used in [1] in the case of regression equations. Only for finding the equation (2), a system of four equations should be solved.

Let $t = (t_1, t_2, ..., t_n)$, $x = (x_1, x_2, ..., x_n)$. Then the scalar product of the vector $(t, x) = t_1x_1 + t_2x_2 + ... + t_nx_n$. Thus a system of equations would be as follows:

$$\begin{cases} a(t,t) + b(t,x) + c(t,z) = (t,y) \\ a(x,t) + b(x,x) + c(x,z) = (x,y) \\ a(z,t) + b(z,x) + c(z,z) = (z,y) \\ \sum_{i=1}^{n} (at_i + bx_i + cz_i + d) = \sum_{i=1}^{n} y_i \end{cases} \tag{4}$$

while in case of seeking the equation (3), a system of seven equations should be solved. Let us write down $at_i + b = t'_i$, $cx_i + f = z'_i$, $ez_i + f = z'_i$, $g - y_i = y'_i$.

Having solved the system (4), we get the coefficients a, b, c and d, of the equation (2) while the solution of a system of equations (5) will allow us to obtain the coefficients a, b, c, d, e, f and g of the equation (3). Based on the above equations (2) or (3), sufficiently reliable forecasts may be made as to what values of the function will correspond to the values of variables lying outside the statistical data.

Consequently the expression of the system will be the following:

$$\begin{cases} \sum_{i=1}^{n} t_i^3 t'_i + t_i^2 (x_i x'_i + z_i z'_i + y'_i) = 0 \\ \sum_{i=1}^{n} t_i^2 t'_i + t_i (x_i x'_i + z_i z'_i + y'_i) = 0 \\ \sum_{i=1}^{n} x_i^3 x'_i + x_i^2 (t_i t'_i + z_i z'_i + y'_i) = 0 \\ \sum_{i=1}^{n} x_i^2 x'_i + x_i (t_i t'_i + z_i z'_i + y'_i) = 0 \\ \sum_{i=1}^{n} z_i^3 z'_i + z_i^2 (t_i t'_i + x_i x'_i + y'_i) = 0 \\ \sum_{i=1}^{n} z_i^2 z'_i + z_i (t_i t'_i + x_i x'_i + y'_i) = 0 \\ \sum_{i=1}^{n} (bt_i + dx_i + fz_i + y'_i) = 0 \end{cases} \tag{5}$$

4. Reliability of forecasts in transportation

The analysis of the transportation development forecasts for the years 1999, 2000, 2005, 2010 and 2015 contained in [2], which were obtained by the methods described in [1], and their comparison with actual statistical data for 1999 and 2000, allowed summarising the data and making some conclusions.

1. The forecasting error for the time series containing the statistical data for the years 1992–1998, which remained unchanged, ranged from 1 % to 10 %. This error is very small; therefore, the forecasts are quite reliable.

2. The errors of forecasting in the time series of statistical data for the years 1992–1998, which changed because of the calculation methods used by Eurostat, range from 25 % to 50 %. These errors are very large; therefore the forecasts cannot be reliable.

3. The effect of the gross national product (GNP) and time factors [8] is best reflected in the time series referring to freight volume and turnover. For example:

The forecast of freight turnover in air transportation for 1999–2015 (in millions of tons per kilometre: mln. ton-km), taking into account the time and GNP variations

1992	1993	1994	1995	1996	1997	1998	1999	2000	2005	2010	2015
Statistical data						Forecast					
6.0	5.0	8.0	4.0	3.0	3.5	3.3	4.04	4.15	4.32	5.39	6.54
6.6	5.0	8.0	4.0	3.0	4	3	3.5	4			

The following regression equation is used in the forecast:

$$\hat{y} = (-7.288E-08)t_i^2 + (-0.2691823)t_i + (3.3E-09)x_i^2 + (5.02E-16)x_i + 2.32,$$

where t_i is the time factor of transportation development trends, while x_i is the factor associated with GNP, $-7.288E-08 = -7.288 \cdot 10^{-08}$, for all the equations given below.

The forecast of freight turnover in railroad transportation for 1999–2015 (mln. ton-km), taking into account the time and GNP variations

1992	1993	1994	1995	1996	1997	1998	1999	2000	2005	2010	2015
Statistical data						Forecast					
11337	11030	7996	7220	8103	8622	8265	9099	9316	9777	11717	13798
11337	11030	7996	7220	8103	8622	8265	7849	8919			

The following regression equation is used in the forecast:

$$\hat{y} = (-6.485E-07)t_i^2 + (-408.841)t_i + (5.46E-06)x_i^2 + (3.8E-13)x_i + 6076.19.$$

The forecast of freight transportation by air for 1999 – 2015 (in thousands of tons), taking into account the time and GNP variations

1992	1993	1994	1995	1996	1997	1998	1999	2000	2005	2010	2015
Statistical data						Forecast					
3.3	2.8	4.4	2.6	1.9	2.8	2.8	3.30	3.43	3.85	4.98	6.18
3.3	2.8	4.4	2.6	1.9	2.8	2.8	3.0	3.3			

The following regression equation is used in the forecast:

$$\hat{y} = (-7.27E-08)t_i^2 + (-0.159715)t_i + (2.648E-09)x_i^2 + (5.03E-16)x_i + 1.628.$$

The forecast of freight transportation by sea for 1999–2015 (mln. tons), taking into account the time and GNP variations

1992	1993	1994	1995	1996	1997	1998	1999	2000	2005	2010	2015
Statistical data						Forecast					
5.1	5.5	4.9	5.8	4.7	4.5	4.2	4.96	5.02	5.20	5.64	6.37
5.1	5.5	4.9	5.8	4.7	4.5	4.2	4.3	4.5			

The following regression equation is used in the forecast:

$$\hat{y} = (-7.287E-08)t_i^2 + (-0.251872)t_i + (2.641E-09)x_i^2 + (5.02E-16)x_i + 3.773.$$

The forecast of freight transportation by water for 1999 – 2015 (mln. tons), taking into account the time and GNP variations

1992	1993	1994	1995	1996	1997	1998	1999	2000	2005	2010	2015
Statistical data						Forecast					
6.5	6.2	5.5	6.3	5.3	5.2	5.4	5.4	5.5	5.8	6.5	7.6
6.5	6.2	5.5	6.3	5.3	5.2	5.5	5.1	5.4			

The following regression equation is used in the forecast:

$$\hat{y} = (-7.292E-08)t_i^2 + (-0.285237)t_i + (3.3E-09)x_i^2 + (5.01E-16)x_i + 3.74.$$

4. The time series referring to the forecast of the volume of passengers and their turnover reflects the effect of GNP and time factors only to small extent. For example:

The forecast of passenger transportation by Lithuanian public transport for 1999–2015 (mln. passengers), taking into account the time and GNP variations

1992	1993	1994	1995	1996	1997	1998	1999	2000	2005	2010	2015
Statistical data						Forecast					
997.1	816.5	788.5	694.7	593.1	532.3	514.8	591.5	622.5	710.7	957.5	1219
997.1	816.5	788.5	694.7	609.4	551.4	516.2	471.9	383.2			

The following regression equation is used in the forecast:

$$\hat{y} = (-1.223E-08)t_i^2 + (-36.07968)t_i + (5.854E-07)x_i^2 + (-1.8E-16)x_i + 228.665.$$

The forecast of passenger transportation by public road transport for 1999–2015 (mln. passengers), taking into account the time and GNP variations

1992	1993	1994	1995	1996	1997	1998	1999	2000	2005	2010	2015
Statistical data						Forecast					
973.0	789.9	768.1	676.0	578.0	519.4	502.2	560.8	586.4	653.4	863.7	1087
973.0	789.9	768.1	678.2	593.55	537.1	502.1	458.3	372.7			

The following regression equation is used in the forecast:

$$\hat{y} = (-1.209E-07)t_i^2 + (-35.09)t_i + (5.286E-07)x_i^2 + (-1.9E-16)x_i + 245.792.$$

The forecast of passenger transportation by bus for 1999 – 2015 (mln. passengers), taking into account the time and GNP variations

1992	1993	1994	1995	1996	1997	1998	1999	2000	2005	2010	2015
Statistical data						Forecast					
646.9	509.1	481.5	405.7	361.6	346.8	316.3	350.2	386.9	426.4	554.7	691.5
646.9	509.1	481.5	405.7	361.6	346.8	316.3	273.5	213.3			

The following regression equation is used in the forecast:

$$\hat{y} = (-1.032E-07)t_i^2 + (-22.238668)t_i + (3.28E-07)x_i^2 + (-3.1E-16)x_i + 178.155.$$

The evaluation of the effects of the GNP and time factors is most relevant to forecasting the above parameters.

5. The research conducted has demonstrated that the most reliable forecasts may be made when the methods of choosing the proper non-linear regression equation described in Section 2 of the present paper are used.

5. Methods of using multidimensional regression and correlation analyses in transportation

Supposing that the value y_1 of the economic index considered corresponds to a set of particular characteristics $(x_1, z_1, ..., t_1)$ of the variables $x, z, \ldots, t$, while the value y_n corresponds to the *n-th* set $(x_n, z_n, ..., t_n)$. Then, the relationship between the variables $(x_i, z_i, ..., t_i)$ and the considered value y_i may be functional or correlation. If y is any economic index of transportation, when $x, z, \ldots, t$ are gross national output, national income, volume of output, etc, and time spaces, then having found the analytical expression of the relationship $y = f(x, z, ..., t)$ between the set $(x, z, ..., t)$ and the index considered, we may determine the values of y for several periods of time in future. In the simplest case, if we suppose that there exists relationship between three variables t, x, y (i.e. t – time spaces, x – gross national output and y – freight turnover), and if this relationship is linear, then:

$$y' = at + bx + c. \tag{6}$$

If the relationship is not linear, but of the second degree, then:

$$y'' = at^2 + at + cx^2 + dx + e. \tag{7}$$

The problem arises of calculating the parameters a, b, c of the regression equations (6) or the parameters a, b, c, d, e of (7).

This problem may be solved by the least square method implying that such parameters of regression equations should be found that the analytical values of y have minimal deviation from actual statistical data y_i^* values:

$$S = \sum_{i=1}^{n} (y_i - y_i^*)^2 \to \min.$$

Substituting the expressions (5) or (6) for y we will get the following:

$$S_1 = \sum_{i=1}^{n} (at_i + bx_i + c - y_i^*)^2 \to \min$$

or

$$S_2 = \sum_{i=1}^{n} (at_i^2 + bt_i + cx_i^2 + dx_i + e - y_i^*)^2 \to \min.$$

Differentiating S_1 with respect to a, b, c or S_2 with respect to a, b, c, d, e as well as equating parts of the derived value to zero (finding the extremum) a system of equalities will be obtained for the linear relationship (8) and for non-linear relationship (9) from the following correlation table:

t	t_1	t_2	…	t_n
x	x_1	x_2	…	x_n
y	y_1	y_2	…	y_n

$$\begin{cases} a\sum_{i=1}^{n} t_i^2 + b\sum_{i=1}^{n} t_i x_i + c\sum_{i=1}^{n} t_i = \sum_{i=1}^{n} y_i t_i \\ a\sum_{i=1}^{n} t_i x_i + b\sum_{i=1}^{n} x_i^2 + c\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i x_i \\ a\sum_{i=1}^{n} t_i + b\sum_{i=1}^{n} x_i + nc = \sum_{i=1}^{n} y_i \end{cases} \tag{8}$$

$$\begin{cases} a\sum_{i=1}^{n} t_i^4 + b\sum_{i=1}^{n} t_i^3 + c\sum_{i=1}^{n} t_i^2 x_i^2 + d\sum_{i=1}^{n} t_i^2 x + e\sum_{i=1}^{n} t_i^2 = \sum_{i=1}^{n} y_i t_i^2 \\ a\sum_{i=1}^{n} t_i^3 + b\sum_{i=1}^{n} t_i^2 + c\sum_{i=1}^{n} t_i x_i^2 + d\sum_{i=1}^{n} t_i x_i + e\sum_{i=1}^{n} t_i = \sum_{i=1}^{n} y_i t_i \\ a\sum_{i=1}^{n} t_i^2 x_i^2 + b\sum_{i=1}^{n} t_i x_i^2 + c\sum_{i=1}^{n} x_i^4 + d\sum_{i=1}^{n} x_i^3 + e\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} y_i x_i \\ a\sum_{i=1}^{n} t_i^2 x_i + b\sum_{i=1}^{n} t_i x_i + c\sum_{i=1}^{n} x_i^3 + d\sum_{i=1}^{n} x_i^2 + e\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i x_i \\ a\sum_{i=1}^{n} t_i^2 + b\sum_{i=1}^{n} t_i + c\sum_{i=1}^{n} x_i^2 + d\sum_{i=1}^{n} x_i + ne = \sum_{i=1}^{n} y_i \end{cases} \quad (9)$$

Solving the system of equations (8) we will calculate the equation (7) coefficients a, b, c, d and e. Basing on the obtained equations (6) or (7) it is possible to predict quite accurately which values of the function will correspond to the values of variables which lie beyond the statistical data, belonging to some time periods in future.

When calculating y values for any $t_{n+1}, t_{n+2}, ..., t_{n+p}$ we are faced with the problem how to find the values of $x_{n+1}, x_{n+2}, ..., x_{n+p}$ because we do not know them. This problem may be solved in two ways:

1. Predicting these values based on expertise or the heuristic methods;

2. Predicting these values using the two-dimensional regression equation $x = f(t)$ and the available data correlation tables.

When choosing the analytical expression (trend) of the function (in our case, linear (6) and non-linear (7) relations are found, which are then compared to establish which one more accurately represents the relation between y^* and $f(x,t)$. In our case two different analytical expressions (6) and (7) of the functions $f(x,t)$ have been found. Statistical data (from the correlation table) are consequently supplemented with the calculated y_i' and y_i'' values.

t	t_1	t_2	…	t_n
x	x_1	x_2	…	x_n
y	y_1	y_2	…	y_n
y'	y_1'	y_1'	…	y_1'
y''	y_1''	y_2''	…	y_n''
$(y-y')^2$	$(y_1-y_1')^2$	$(y_2-y_2')^2$	…	$(y_n-y_n')^2$
$(y-y'')^2$	$(y_1-y_1'')^2$	$(y_2-y_2'')^2$	…	$(y_n-y_n'')^2$

The following calculations are made:

$S_1 = \sum_{i=1}^{n} (y_i - y_i')^2$ and $S_2 = \sum_{i=1}^{n} (y_i - y_i'')^2$.

If $S_1 < S_2$, then the analytical expression $y' = at + bx + c$ is more accurate, whereas if $S_2 < S_1$, the expression $y'' = at^2 + bt + cx^2 + dx + e$ is more accurate.

However, in some cases, prognostic calculations [1] that have been made according to the techniques discussed do not provide the required degree of accuracy. Therefore, some methods of finding a correlation coefficient or correlation relationship should be used. When a linear regression equation [5] is used in making predictions, then, by adding a row representing the difference between analytical and

empirical y_i values to the correlation table, the correlation coefficient may be found from it. If its value is about zero, this means that the linear regression equation is acceptable for prediction, while if the correlation coefficient equals 0.5 or is higher, another analytical expression of $y = f(x,t)$ should be chosen. Using modern application packages (Excel, Statgraphics, etc.) it is possible to obtain accurate prediction results by means of mathematical simulation. This implies that such analytical expression of the function $y = f(x,t)$ is chosen that the correlation coefficient of the difference between analytical and empirical *y* values of a new time row approach zero. The same technique may be applied in case of the non-linear regression equation (7) used in prediction except that the correlation showing the relationship between non-linear y and x, t is determined here.

Conclusions

♦ The application of the suggested techniques reveals that the non-linear regression equation corresponds more accurately to actual statistical data, thereby allowing a more accurate prediction to be made.

♦ The *suggested* prediction methods deal only with the effect of two factors x and t on the resulting index y, however, these techniques may be expanded to include some more factors $x, z, \ldots, t$.

♦ It would not be reasonable to use the functions $y = f(x, z, ..., t)$ with a very large number of parameters in predictions, since trend equations obtained in this way (particularly, with a small number of observations) will show some random deviations rather than the main trend of development.

References

[1] Mazūra M. (2002) Predicting Major Trends of Transportation Development. *Transport Engineering* **21**, No 2, 57-59.
[2] Baublys A., Griškevičienė D., Žvaliauskas A. (1999) Prognozation of Transport Activity. Lithuania science. *Lithuania Academy of Science Book* **22.** TRANSPORT. Vilnius, 9-61.
[3] Reiman M. I., Rubio R. and Wein L. M. (1999) Heavy Traffic Analysis of the Dynamic Stochastic Inventory-Routing Problem. *Transportation Science* **33**, 361-380.
[4] Yang W.-H., Mathur K., and Ballou R. H. (2000) Stochastic Vehicle Routing Problem with Restocking (2000) *Transportation Science* **34**, 99-112.
[5] Yang H. (1999) System Optimum. Stochastic User Equilibrium and Optimal Link Tolls. *Transportation Science* **33**, 354-360.
[6] Fumero F., Vercellis C. (1999) Synchronized Development of Production. Inventory and Distribution Schedules. *Transportation Science* **33**, 330-340.
[7] Miller-Hooks E. D., Mahmassani H. S. (2000) Least Expected Time Paths in Stochastic Time – Varying Transportation Networks. *Transportation Science* **34**, 198-215.
[8] Baytman P., Erdain A. (1965) *The Higher Transcendental Functions.* Moscow: Nauka. 343 p. *(In Russian)*

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DISTANCE LEARNING FOR SPECIALITIES BELONGING TO MECHANICAL ENGINEERING

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The paper presents experience of activity of Sumy State University aimed at preparation and implementation of distance learning for specialities belonging to mechanical engineering, development of corresponding learning and methodical materials, description of technical and organizational aspects of this activity. The paper presents also the authors' vision concerning future development of modern forms of education of specialists of technical profile.

Keywords: *distance learning, mechanical engineering*

1. Introduction

The last decade was featured with rapid development of information technologies, perfection of personal computers, enlargement of Internet, increase of volume and rate of data exchange via World Wide Web, as well as reduction of prices for corresponding equipment and communication services. All this opens new possibilities for very different spheres of human activity and, in particular, for education.

Modern computer and Internet technologies suggest new technical possibilities for creation of more effective and obvious learning materials that help in easier and more profound understanding of new knowledge, simplify delivering of learning materials and organizing of feedback, enabling students to receive quicker responses for their questions [1]. These new possibilities require consideration and development of corresponding methodical basis in order to make the teaching process to become as efficient as possible.

Taking this into account, last years Sumy State University (SumSU) deals with development and perfection of modern learning and methodical materials with the purpose to improve quality of education process. This paper describes some experience of the university concerning preparation for implementation of distance learning in the specialities belonging to mechanical engineering. The reason for selection of these specialities is due to increasing demand for engineers in our country and the fact that the students of these specialities should master large volumes of complex material, thus, application of modern information technologies in this sphere can be very helpful.

Successful fulfilment and implementation of this work in the teaching process should be promoted by the fact that many engineering faculties of SumSU occupy leading positions in their fields. Besides, the university has longstanding experience in teaching in disciplines of mechanical engineering and the team of qualified lecturers and research scientists.

2. Preparation of distance learning for specialities belonging to mechanical engineering

2.1. CREATION OF A LIBRARY OF E-MANUALS

Providing students with manuals is a problem that always faced institutes of higher education. Last years this problem is especially urgent due to rapid development of science, especially relating to information technologies. Due to large cost prices of printed books, the possibilities to provide students with manuals are somewhat restricted. At the same time, at the contemporary stage of development of information technologies, new ways of distribution of information are widely used – as electronic files written on CDs (compact discs) or published at Internet sites [1]. Distribution of information in electronic form is much cheaper than in printed form. Besides, modern technologies provide authors of e-manuals with possibilities to use audiovisual interactive media, allowing for improvement of appearance and contents of manuals and effectiveness of mastering new information.

Nowadays, a lot of universities all over the world prepare electronic learning courses written on CD to transfer them to students. Due to large capacity of a standard CD, it is convenient to write on one or several CDs all the learning courses that students should master during their studying, and give these CDs to students after their admittance to the university. Thus, the students will seldom need to visit libraries, only when they require books not included to basic learning courses presented at CD.

In Sumy State University, a separate scientific group, in conjunction with lecturers of engineering and other faculties, deals with development of library of such e-manuals and corresponding methodical materials for students of specialities belonging to mechanical engineering. At present, the e-library includes all the courses relating to the first three years of study for specialities of mechanical engineering (approx. 2 dozens of courses), as well as all the methodical materials edited in the university during last several years. We consider the creation of such a library to be the necessary stage prior to organization of distance form of learning, as this distance learning assumes that all the learning and methodical materials are delivered to students in electronic form.

2.2. DISTANCE FORM OF LEARNING

A consequence of development of modern technologies is possibility for effective organization of distance learning, i.e., when a teacher and a student can exchange with information, being located at a large distance one from another. Of course, distance form of learning can not fully reproduce the experience gained by internal students during personal communication with teachers and other students during practical training and laboratory works. Besides, distance education assumes that students are motivated highly enough and able for purposeful self-dependent work. Distance form of study has much in common with external from, with the difference that a distant student receives all the learning and methodical materials in electronic view – via CD, e-mail or Internet. At the same time, distance form of study has a number of essential advantages:

1. Students are not required to visit the university in person, except for during exam sessions. Everything that students need for work is a computer connected to the Internet. As a consequence, both direct and indirect expenses, both for students and the university, at distance form of learning are quite low.
2. Students can study at any convenient time, being located at any place of the planet. Moreover, distance form of study permits to organize the educational process to be as flexible and individualized as possible, taking into account real demands and level of preparation of separate students.
3. It is possible to review regularly the contents of distance courses and supplement them with new information materials. It is rather important, taking into account quick obsolescence of information in many courses nowadays.
4. After finish of study, a student keeps all the electronic lectures, e-manuals and other learning and methodical aids forever. At present, as a rule, even the internal students can hardly take advantage of this.
5. Distance learning is the only acceptable form of study for a number of persons who live far from the university centres, as well as for persons with restricted physical capabilities.

In SumSU, we have the laboratory of distance learning that deals with development of e-manuals and computer simulators. At present, the laboratory has developed 49 distance courses that are taught at the 1st, 2nd and 3rd years of study according to the curriculum of the speciality “Economics”, 1st and 2nd years of study of the speciality “Information Science” and 1st year of study of the speciality “Mechanical Engineering”. At present, several “pilot” groups of students use these courses in education. Lecture materials of the developed electronic courses are mostly made as sets of *HTML*-pages or *PDF*-files interconnected by cross-references. In the paper [2], the structure of the developed electronic courses is described in more detail. The features of the separate electronic courses are described in the chapter 3.

2.3. ORGANIZATIONAL ASPECTS OF PREPARATION OF THE LEARNING AND METHODICAL MATERIALS

The author of each learning course is the lector of this course. As creation of a distance course is a labor consuming process, the university concludes a treaty with the lector concerning creation of the course, with the payments delivered after each stage of the treaty. The university engages also the students to help the teachers to prepare materials for the distance course. After composing of an e-course, its texts are printed and than checked and corrected at the editorial department of the university. Later, e-courses are gradually improved by adding high-quality figures, fresh links to Internet sites, etc.

3. Technical aspects of preparation of the learning and methodical materials

3.1. EXPERIENCE CONCERNING CREATION OF SEPARATE E-COURSES

Electronic courses related to humanities are relatively easy to create, as they contain mainly static text. Text of such e-courses is prepared in *HTML*-format. The disc volume occupied by such a learning course, as a rule, does not exceed 1 – 2 Mb. Later, of course, it would be expedient to improve their design and fill them with illustrations, in order to make them more pleasing for study. E-course of descriptive geometry and engineering graphics, as well as a number of courses of designing in mechanical engineering, are featured with a high number of figures in lectures. At the laboratory of distance learning of SumSU, the technology for creation of such figures by means of vector graphics was developed [3]. The advantages of formats of vector graphics (*SVG*, *SWF*, *VRML*) are high quality of images, availability of zooming feature, relatively small size, possibility for creation of animated cartoons as well as active objects that can react on the actions of a user.

As a tool for preparation of such figures, any package for designing in mechanical engineering can be used – *AutoCAD, SolidWorks*, etc. (see [4]). These packages can save the models in formats suitable for representation of the objects directly at the Web page, using standard browsers. For this purpose, as a rule, only a small freely available plug-in viewer should be downloaded. In particular, *SVG*-format is very convenient for preparation of the industrial drawings and their publication in the Internet, *VRML*-format – for creation of 3D objects, with the possibility to examine them from different viewpoints. Files of *SWF*-format are created using the software tool *Macromedia Flash*. This tool is a prefect choice for creation of the 2D animated cartoons reacting on user actions.

In order to ensure proper self-instruction of students, in particular, in descriptive geometry and engineering graphics, it would be expedient to create a problem simulator, where a student is proposed to fulfil various assignments concerning construction of absent lines, surfaces, projection views, etc. E-simulator, implemented as a software tool, would supply a student with proper interface for performing these constructions, check their correctness, indicate errors and grade the student, without assistance of a teacher. Such a simulator, implemented as a software tool for DOS, was developed, in particular, in Ufa State Aviation Technical University, its demo-version can be downloaded at http://www.ugatu.ac.ru/ddo/courses.htm.

E-manuals of higher mathematics, physics, etc., are featured with very large number of formulas, as well as rather large number of figures. The lectures of such courses are prepared in *PDF*-format. This format ensures independence of appearance of lectures, including splitting into pages, on the computer platform, convenience of printing and possibility to create documents with complex formatting (including figures, formulas, etc.). At the laboratory of distance learning of SumSU, a set of e-simulators was developed. These simulators are appeared at a web page as *Java*-applets and provide students with interactive assistance during the process of fulfilment of the various assignments, and check the correctness of fulfilment [5]. This set of simulators is found at the site http://dl.sumdu.edu.ua and used in the educational process in Sumy State University.

3.2. APPLICATION OF MODERN SOFTWARE PACKAGES FOR DESIGNING IN MECHANICAL ENGINEERING IN TEACHING OF ENGINEERING DISCIPLINES

The designing in mechanical engineering is one of the spheres of human activity where implementation of computers and modern software permits to save huge volume of manual labor and increase quality of the obtained results. It is impossible to imagine designing activity at modern engineering enterprises without application of computers and relating software. The review of these packages is presented in [4]. Getting experience of work with such software is important aspect in preparation of a modern engineer, that’s why, in our university, practical work with this software packages is included in the curriculum.

The first discipline where the students become familiar with the basics of work with these packages is the engineering and computer graphics that is mastered at the first year of study. Then these packages can be applied in practice during preparation of the course project in machinery. Later these packages can be used for preparation of course project in special disciplines (designing of pumps, turbines, compressors, lathes, chemical reactors, etc. – according to particular speciality), and then for preparation of the graduate project. Here, it is expedient to accumulate the projects performed by students, together with accompanied documentation, in a database. Then the subsequent groups of students will be able to use it for preparation of their own course and graduate projects, and the teachers

will be able to pose them more complex problems. Implementation of these software packages in the teaching process for study of designing in mechanical engineering is expedient also at the distance form of study. It would be helpful for a distant student to obtain a CD filled not only with e-manuals and methodical aids, but also with database of design projects prepared by the previous groups of students. These packages allow for students and teachers of distance form of study to organize preparation of course and graduate projects in electronic form that will permit to prepare qualified specialists.

3.3. APPLICATION OF MODERN SOFTWARE PACKAGES FOR FLUID FLOW SIMULATION IN TEACHING OF THE ENGINEERING DISCIPLINES

At many specialities of mechanical engineering, the courses of fluid mechanics are provided and processes related to fluid flows in different technical and industrial devices are studied. Modern level of development of information technologies allows for creation and implementation of E-manuals and simulators that by use of visual aids assist significantly in learning of these disciplines. During last years, for prediction of many natural phenomena, as well as designing of different technical devices, numerical methods of simulation of fluid flows implemented in modern software tools are successfully used. The reviews of such software tools and their capabilities are presented, e.g., in [6–8]. Evidently, besides the main destination of such software, i.e., prediction of characteristics of fluid flows, such software tools can be used in educational purposes, for illustration and analysis of typical simple flows, as well as flows occurring in different technical devises [9]. Creation and implementation of e-manuals using this software allows for improvement of presentation of materials by visual aids and assists significantly in mastering of these disciplines.

Again, it is expedient to accumulate the projects performed by students in a database for use by subsequent groups of students, also at distance form of study. It would be helpful for a distant student to obtain a CD filled with database of projects prepared by the previous groups of students.

3.4. SOFTWARE TOOL FOR TESTING OF KNOWLEDGE WITH ELEMENTS OF FUZZY LOGICS

For convenience of composition and conduction of tests, as well as well-ordered storage of test results, a special software tool, *SSUquestionnaire*, was developed in Sumy State University [10, 11]. This software tool allows for a teacher not familiar with modern information technologies to prepare tests easily according to any available type and present them as a multi-frame page for a web browser. Demo-version of this software tool is exposed at the address http://dl.sumdu.edu.ua/ssuquest.html.

The software tool *SSUquestionnaire* features with a special flexible algorithm for evaluation of knowledge. Firstly, a fuzzy logic approach implemented in this tool allows students to indicate how much they are sure in their answers [12]. The higher is the confidence level declared by a student, the more point he will obtain provided the answer happens to be correct and the more points he will loose in case of wrong answer. Secondly, the algorithm for computation of points earned by students provides a technique for computation of relative complexity of test questions. Thus, each question of the test is assigned a certain “price”, i.e., number of points a student can earn for the correct answer.

Conclusion

Thus, in Sumy State University, some experience for performing of the organizational and methodical work aimed at preparation for implementation of distance learning of students in specialities belonging to mechanical engineering was accumulated. This work aims at improvement of quality of educational process during the whole period of preparation of the specialists in mechanical engineering.

References

[1] Alexeyev A. N., Volkov N. I. (2002) *Computer in the teaching process of higher school.* Sumy: Dovkillya. 389 p. (In Russian)

[2] Alexeyev A. N., Volkov N. I., Kochevsky A. N. (2004) Creation of a library of E-manuals for students of mechanical engineering with tests based on fuzzy logic. *Bulletin of the Petroleum and Gas University of Ploiesti- Ploiesti (Romania)* **1**, 42-46.

[3] Kochevsky A. N., Piven A. G., Slepushko N. Yu. (2004) Modern Formats of Vector Graphics for Distance Courses in Engineering Disciplines. *Proceedings of the Fourth International Conference “Internet-Education-Science-2004”, September 28-October 16, 2004, Vol. 1.* Vinnytsia, 228-229.

[4] Volkov N. I., Alexeyev A. N., Kochevsky A. N. (2004) Review of modern software packages for designing in mechanical engineering and their application for teaching engineering courses. *Science and education: Proceedings of papers.* Kharkov: NTU "KhPI", 347-350. (In Russian)

[5] Lugovoy N. N., Lyubchak V. A., Sobaeva E. V. (2003) Unit of interactive cognitive activity in the system of distance *learning*. *Education and Virtuality*, ***7***. Kharkov-Yalta: UADO, KhNURE, 296-299. (In Russian)

[6] Kochevsky A. N. (2004) Computation of internal fluid flows in channels using the CFD software tool FlowVision, http://arxiv.org/abs/physics/0409020.

[7] Kochevsky A. N., Nenya V. G. (2004) Contemporary approach for simulation and computation of fluid flows in centrifugal hydromachines. *Bulletin of the Petroleum and Gas University of Ploiesti – Ploiesti (Romania)* **2**, 22-37. (Also published at the International arXiv.org e-Print archive), http://arxiv.org/abs/physics/0409102.

[8] Kochevsky A. N. (2004) Possibilities for simulation of fluid flows using the modern CFD software tools, http://arxiv.org/abs/physics/0409104.

[9] Volkov N. I., Alexeyev A. N., Kochevsky A. N. (2004) Modern CFD software tools and their application in the studying process, *Information technologies in education, science and engineering – Materials of the IV All-Ukrainian conference of young scientists ITONT-2004, Pt. 2.* Cherkassy: ChNU, 84-87. (In Russian)

[10] Volkov N. I., Alexeyev A. N., Kochevsky A. N. (22.04.2004) Software tool "SSUquestionnaire", *Registration Copyright Certificate on the Work, No. 9856*, Ministry of Education and Science of Ukraine, State Department of Intellectual Property, Kyiv. (In Ukrainian)

[11] Alexeyev A. N., Volkov N. I., Kochevsky A. N. (2004) Technique for composition of tests using the software tool SSUquestionnaire. *Higher Education Perspectives: The Role of Inter-University Consortia: Proceedings of International Scientific Conference*. Mykolaiv: Atoll, 12-14. (In Russian)

[12] Alexeyev A. N., Volkov N. I., Kochevsky A. N. (2003) Elements of fuzzy logic in computer-aided control of knowledge. *Open Education* **4**, 23-25. (In Russian)

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USING COUNTER PROPAGATION NEURAL NETWORK FOR BUILDING INTELLECTUAL DECISION SUPPORT SYSTEMS

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Commonly, complex modern manufactures systems' controlling makes its operators pass important decisions what sometimes is rather difficult when there are many alternatives. Such situation requires developing and involving of automatic intellectual decision support systems (DSS). Different approaches have been already developed in order to help operator with passing correct decisions. Each has its advantages and disadvantages.

This work presents a new approach to building decision support systems based on modified counter propagation neural network. Intellectual self-training automatic control systems and intellectual self-training decision support systems allow switching from old subjective methods of manual control to up to date intellectual informational control technologies for badly formalized processes and objects functioning under uncertain conditions. The following main tasks of the presented work have arisen from this assertion.

Keywords: *automatic intellectual decision support systems*

1. Target setting

The developed system is supposed to be able to recognize current state of a controlled process or object giving corresponding instructions on control influence. The system must be capable of self-training while being utilized. The system is supposed to be able to be trained even on small data sets. The system must store data it receives for further after-training.

More specifically the system must determine which class the current state belongs to and display instructions related to that class. This can be done with the help of training data set clustering and constructing of classes putting each data cluster into a hyper-sphere that represents a subclass. An expert who analyses the set of subclasses created by the system during training process unites subclasses into classes and writes instructions related to each class. Using subclasses for constructing classes allows creating classes with borders that are more accurate and in most cases avoiding classes' intersection.

2. DSS structure development

Controlled process or object current state recognition block has been placed at the heart of the system (Fig. 1). The task of this block is recognizing the controlled process or object current state. For this purpose a counter propagation neural network has been used and then subjected to certain changes.

The chosen neural network type is capable of training using small datasets; can be trained while being utilized improving its operational quality; can operate and be trained with high speed. In addition using neural networks doesn't require profound investigation of the controlled process or object nature.

The current state recognition block has been associated with a database containing descriptions of studied controlled process or object states and instructions related to them. In this way the system can recommend operator to perform some actions to improve the controlled process or object current state that is to bring the controlled process or object closer to its ideal state, which doesn't require any control actions.

At the training stage while the subclasses are not completely formed yet there are a lot of unrecognised input data vectors. Such data vectors are stored in database and periodically the system is retrained to form new subclasses and change the old ones — training without teacher. After that expert analyses the data and relates the subclasses to different classes (already existing or new) forming complex structure classes (Fig. 2).

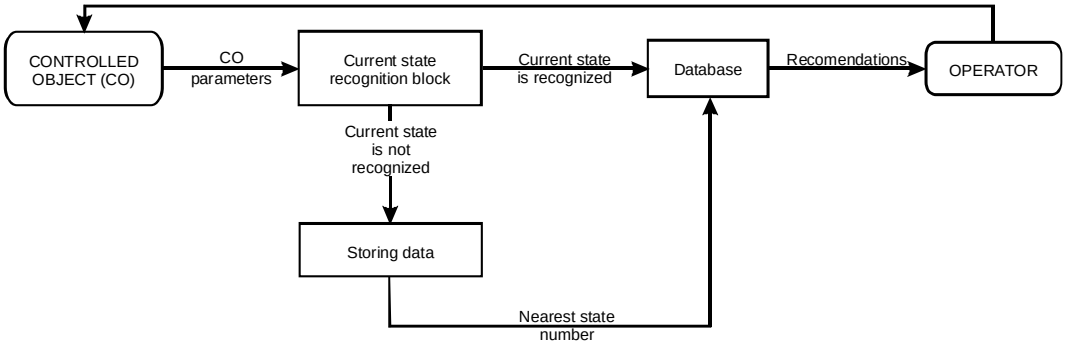

Figure 1. DSS structure

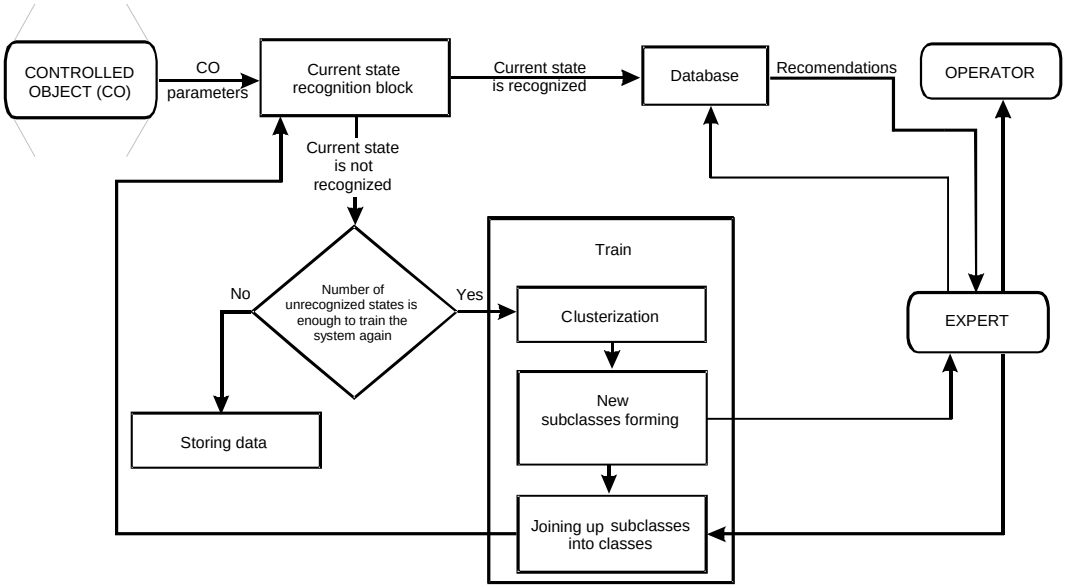

Figure 2. DSS training

3. Recognition block functioning principles development

The counter propagation neural network contains so-called Kohonen layer that is commonly used for data clustering. Such a feature suits the best for forming subclasses' centres. In addition all the Kohonen neurons have been provided with extra parameter for subclasses' radiuses simulation.

Each Kohonen neuron has been associated with a subclass that is the system is supposed to find the nearest to input data vector subclass and the related class.

In addition to data classification the neural network must recognize situation when input data vector belongs to none of the existing subclasses and must be capable of retraining to improve the existing subclasses and form new subclasses using new data. This can be done with the help of threshold activation function (Fig. 3) that is not typical for this type of neural networks but still it can be used.

$$F(x) = 1 - \frac{x}{R},$$

R – can be considered as subclass container radius.

Such threshold function also shows relative depth of input within subclasses. This can help to determine what class the input belongs to in case of classes' intersection comparing relative depth of input within subclasses instead of absolute distance between the input and the classes' centres.

To correctly train the network it is necessary to determine optimal initial number of neurons and initial weight value for each neuron of Kohonen layer. Incorrect initial allocation of neurons may cause situation when some neurons which are rather far from data will not be used at all and some neurons will be too close to each other creating set of not intersecting subclasses.

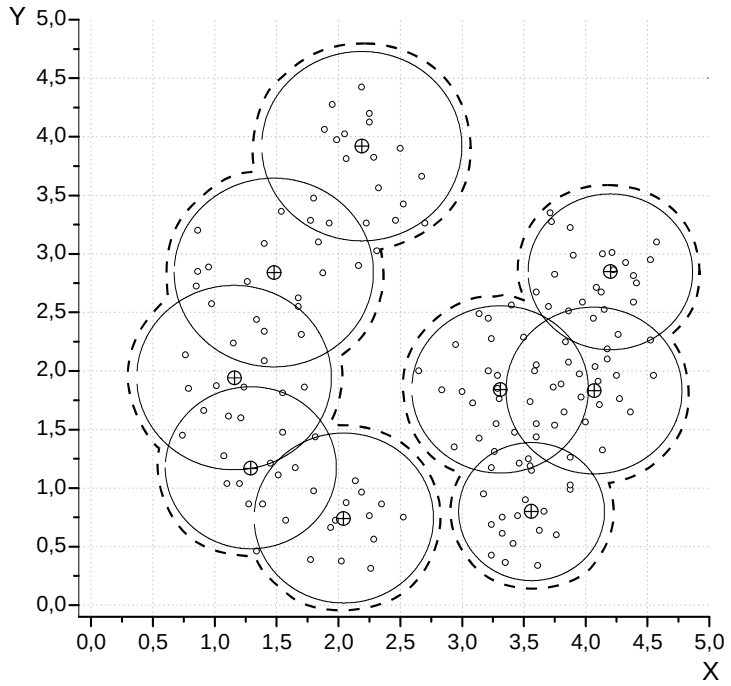

Figure 3. An example of recognition classes' containers forming. Borders of classes (containers) formed joining subclasses are marked with dotted line.
X, Y — parameters of a certain controlled process or object.
O — input parameters vectors (used for training).
⊕ — centers of subclasses (neurons weights vectors after training)

The following approach has been developed for getting an appropriate initial neural network structure and initial Kohonen neuron weights. Initial neurons number must equal the total number of input vectors and initial Kohonen neuron weights are obtained by adding small noise to input vectors. Thus the entire set of initial weights is very close to input vectors. Obviously, there will be a lot of extra neurons in this case and a lot of them will not be used. Such neurons can be eliminated after the first iteration. Yet the total number of neurons can be higher then needed. Such neurons can be eliminated starting from condition that each subclass has to have more then *n* input vectors.

The second so-called Grossberg neuron layer that goes after Kohonen layer is used to build classes from subclasses. Expert uses Grossberg neuron layer to join subclasses into classes. The Grossberg neurons have weights equalling to classes numbers. Thus since only one Grossberg neuron has input that equal to 1 and the rest are 0 the Grossberg layer output equals to the number of class the network input belongs to. This approach allows building much more precise class container borders with the help of set of hyper spheres (Fig. 3). In addition it allows avoiding any possible issues caused by classes' intersections.

Conclusion

Complex technological processes and objects controlling is one of the most common issues of modern manufacture since such processes and objects are characterized with significant amount of information to be analysed before taking any decision. This issue can be solved with the help of decision support systems; besides modern manufacture requires new up-to-date intelligent self-training systems.

In this work it is suggested that controlled process or object current state recognition block based on modified counter propagation neural network is placed at the heart of the DSS in order to recommend some control actions depending on the current state.

It has been ascertained that Kohonen neuron layer of a counter propagation neural network subjected to certain changes can be used for recognition classes (system states) creating in the form of hyper-spheres aggregate in variables space. Such aggregate can describe classes' borders rather well. In addition an algorithm for clustering layer neuron number selection and initial weights generation has been developed and tested.

The approach has been implemented by means of C++ programming language in Borland Builder environment. Object oriented programming has been used in order to create at most flexible tool for holding different numeric experiments and playing with the neural network structure and parameters.

The developed algorithm has been tested at the example of complex fertilizers NPK (nitrogen, phosphorus, and potassium) manufacture operator DSS at JSC "Sumyhimprom".

References

[1] Kohonen T. (1997) *Self-organization and associate memory.* New-York: Springer-Verlang. 428 p.

[2] Ridkokasha A. A., Golder K. K. (2002) *Foundations of systems of artificial intelligence*. Cherkasy: Vidlunnya-Plus. 240 p.

[3] Krasnopoyasovskiy A. S. (2004) *Intellectual control systems informational synthesis: An approach based on functional-statistic trials method.* Sumy: Sumy State University Publishing house. 261 p.

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TEACHING TECHNIQUES IN PROFILE EDUCATION

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The specifications for profile education reflect the objectives of the Information Systems Management Institute curriculum presented in the ”Common European Framework of Reference for Languages: Learning, teaching, assessment”, issued by the Educational Committee of the Council for Cultural Co-operation in 2004 and in the ‘Standards for Modern Foreign Languages’ issued by Latvian Ministry of Education and Science in 1998.

The curriculum defines what language learners have to learn in order to use the language for communication and what knowledge and skills they have to develop so as to be able to act effectively in different domains.

It is very important for the specialists working in the field of modern languages to provide a common basis for the objectives, content and methods applied, to overcome the barriers to communication arising from the different educational systems in Europe, and to enhance the transparency of courses and syllabuses which will facilitate the mutual recognition of qualifications gained in different learning contexts [1].

Keywords: *profile education, competences, communicative language competences, domain, case study, project work*

1. Profile education in language education

Within recent years a great deal of attention has been paid to studying foreign languages at the departments of Information Technologies Management and Business Administration not only in Europe but worldwide. The value of today’s specialists in these spheres is very much determined by their ability to communicate freely with foreign partners, to negotiate with representatives of companies from other countries as well as to read special literature in a foreign language. With Latvia joining the European Union this task has become especially urgent, demanding the revision of the whole educational program in foreign languages.

In 2003-2004 academic year a Project of Profile education in the English language was worked out at the Foreign Languages Department of the Information Systems Management Institute, which was launched in 2004-2005 academic year.

Profile education is a system of training and instruction of young people designed to give knowledge and develop skills in a weighted, reinforced specialty education emphasizing learning in certain directions and producing a ‘profile’ in which a higher level is attained in some areas of knowledge and skill than others, to ensure the students the English language proficiency, familiarity, competence and capacity to use their knowledge effectively for particular purposes of natural communication, reading, writing within the context of the specialty they are majoring in as well as their future personal, occupational, public and educational domains.

In the personal domain, the intention may be to entertain a visitor by exchanging information on families, friends, likes and dislikes, to compare experiences and attitudes, etc. In the occupational domain, it may be to understand new regulations and their implications for a client. In the public domain, it will usually be to transact business, say to buy goods of high quality at reasonable price. In the educational domain, it may be contributed to a role-play or a seminar, or a paper on a specialized topic for a conference or for publication may be written, etc. [1]

Profile education should not be mixed up with English for Specific Purposes (ESP) reflecting rather restricted language areas which might be referred to as either ***modular*** programs of learning, improving the learner’s proficiency in a restricted area for a particular situational purpose or ***partial*** programs, taking responsibility only for certain activities and skills (e.g. reception) and leaving others aside. However, ESP is considered as one of the constituent components of Profile education.

Profile education comprises the vocabulary and language structures of all kinds, not just business terminology. Most of the time, business people are not using special ‘Business English’, they are talking English and using common core vocabulary interspersed with the occasional technical terms (e.g. invoice, consignment). Students should be encouraged to widen all aspects of their English vocabulary, and not just focus on ‘Business English’ vocabulary.

2. Motivational differences in language learning

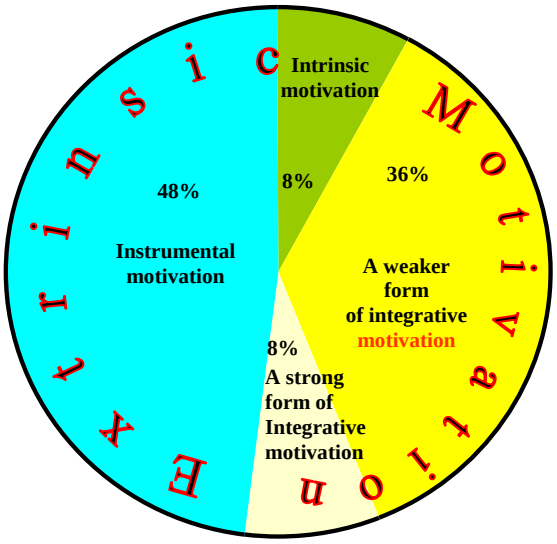

Figure 1. Motivational differences in language learning

All specialists dealing with language teaching know that despite the same circumstances, the same conditions, the teacher and methods applied, some students succeed significantly better than their peers. In the face of such phenomena it seems reasonable to suggest that that the motivation that students bring to class is the biggest single factor, the driving force affecting their success.

The Department of Foreign Languages has done some research into the nature of motivation of the students. What kind of motivation do our students have? We separated it into two main categories: ***extrinsic*** motivation, which is concerned with factors outside the classroom, and ***intrinsic*** motivation, which is concerned with what takes place inside the classroom. The research has given the following results (see, Figure 1).

As it is seen from the pie chart, 92% of students have shown extrinsic motivation. These are students who have long-term goals concerning the language learning.

48% of them possess instrumental motivation, having a belief that mastery of the target language will enhance their chances to get a better job, position, status or will facilitate their professional advancement and help make a good career. The language is an instrument in their attainment of such a goal.

36% demonstrated integrative motivation, being encouraged by the possibility to travel the world, to go on holidays to different countries and the language is seen as a means of communication. Some students are attracted by the culture of the target community and want to know as much as possible about it.

8% of students have a strong form of integrative motivation. These are students who want to pursue their studies at a university in an English-speaking country – in the USA, Canada, Great Britain, or Australia and, ultimately, they wish to integrate into this society.

8% of students bring no extrinsic motivation to the classroom. They may be even apathetic about language learning and study English just because it is in the curriculum, or because their parents consider the knowledge of languages of vital importance. For them what happens in the classroom will be of paramount importance in determining their attitude to the language and in supplying motivation.

What can teachers do about extrinsic motivation and student attitude? It is clear that we cannot create it since it comes into the classroom from outside. It is clear, too, that students have to be prepared to take some responsibility for their own learning. But with that in mind we can still do our best to ensure that students view the language and the learning experience in a positive light. We can do this by creating a positive attitude to the language and its speakers, and we can try to be certain that we are supportive and encouraging to our students rather than critical and destructive. [6]

3. Language skills priorities

Literate people who use language have a number of different abilities. They will be able to speak on the telephone, write letters, watch TV, listen to the radio or read books. In other words they possess the four basic language skills of speaking, writing, listening and reading. Speaking and writing involve language production and therefore often referred to as *productive skills.* Listening and reading, on the other hand, involve receiving messages and therefore often referred to as *receptive skills.*

Very often, of course, language users employ a combination of skills at the same time. Speaking and listening usually happen simultaneously and students may well listen (or read) and write when they make notes.

As we have seen in the previous chapter, there are many different reasons for learning a language, and we have said that we are mainly concerned with a classroom situation in which English is being studied.

We have included both those students who have themselves made the decision to study and also those for whom the study of the language is a compulsory part of their education. Still, having different

types of motivation, what are the skills priorities for the students? What do they hope to be able to do with the language they learn?

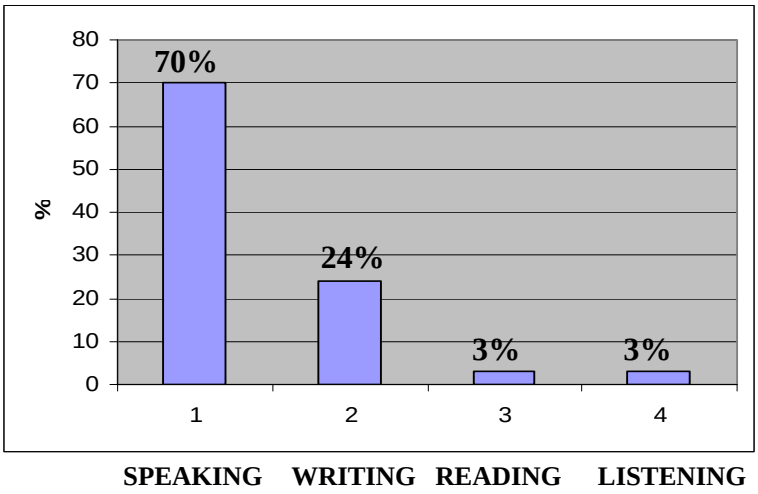

Figure 2. Language skill priorities

According to the bar graph 70% of students hope to become competent speakers and want to develop good conversational skills. 24% of learners consider writing skills important for themselves. Reading and listening are left to take care of themselves, since the students consider they are able to comprehend written and oral messages.

4. The needs of the learners

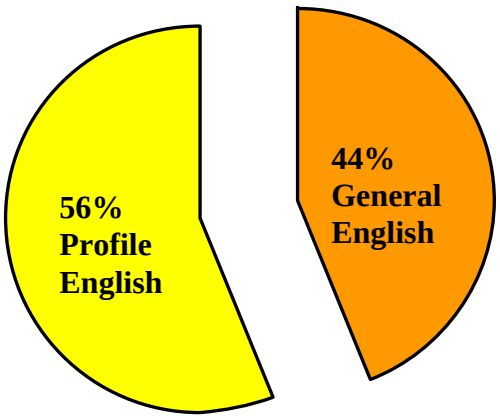

Figure 3. Student needs

Before we decide what kind of practice our class needs, we have to know what they want it for. Is it for passing an exam, writing business reports, working as telephone operators, understanding computer journals, talking to tourists? When planning a syllabus, we therefore have to consider not only language structure, vocabulary and idiom, but also how our students will be using these and why.

56% of students consider that they will be using the language for the purposes of their professional communication. 44% consider that they will be quite satisfied with the knowledge of General English.

Now when we know why the students are learning the language, we are able to specify more or less exactly what they will need to learn both in terms of language and skill. For most students, however, language learning is along-term process, with goals that cannot be satisfactorily defined. Often, when they *are* defined, goals are unrealistic, failing to take into consideration factors such as the amount of time available, classroom conditions, etc. For many students the only reality is final examination with a probable emphasis not on skills that are truly needed but on those that can be measured through a written examination. A poor reward for many years of language learning!

In such circumstances we must try to help the learners in the most realistic way possible. Ultimately, as we have acknowledged, they will need the language for the purpose of communication. How can this best be achieved?

First, it is clear that they must master as much of the language system as they reasonably can: that is, its grammar, its vocabulary and phonology. However, we must remember at the same time that the process should not be boring. What we need are ways of giving the learners only the most essential items of language economically and enjoyably to help them become adequate users of the language.

Secondly, it is equally clear that the learners need opportunities to try out language for themselves: in other words, to experience within the classroom ways of communication through the language. Here again we must keep certain points in mind:

- that communication in the classroom is not quite the same as in 'real life', but this does not mean, of course, that the students will perceive it in this way or that they will benefit less from it;
- that communication will often seem a little less than adequate. The students are all the time learning the language as they try it out and, since we cannot postpone these activities which are essential in building up communication skills, we must be satisfied with what they *try* to do and overlook their shortcomings.

These two goals can be summed up by saying that we would like the learners to be able o use the language both with *accuracy* – which depends on mastery of the language system – and with *fluency* – which derives from experience of trying the language out for oneself. Our task, in trying to meet the needs of learners, particularly in non-privileged classroom conditions, is to strike a balance between these two goals so that, in the end, the learners are able to *communicate adequately*.

5. Prioritising options in teaching technologies

Implementation of teaching technologies, especially in profile education, must have some effect on students' motivation. We have to remember that we deal with adult education and our students are often highly motivated. If they were not they would not see the need to continue with language study. If they find the method deadly boring, they might become de-motivated or just 'switch off', whereas if they have confidence in the method they will find it motivating and can be highly intelligent if stimulated and dedicated if involved. But it seems to be the most difficult area of all to be certain about.

As we have already mentioned, those students who are really motivated, will probably succeed whatever method is used. At the same time different students are more or less sympathetic to any particular method depending upon their expectations. We can easily recall students who felt that there was not enough grammar or enough conversation depending on their taste at the time.

Unfortunately, there is no research which clearly shows the success of one method over another. And what is more, two teachers using the same method can have vastly different results. However, what we do know is that if the student loses confidence in the method, he will become de-motivated. And the student's confidence in the method is largely in the hands of the most important factor affecting motivation – the teacher. [6]

Taking all the aforementioned into account, we attempted the research into the priorities of teaching methods and technologies as viewed by our students in order to find out what kind of activities attract them most and which teaching techniques they sympathize and find effective in language acquisition.

Here are the results:

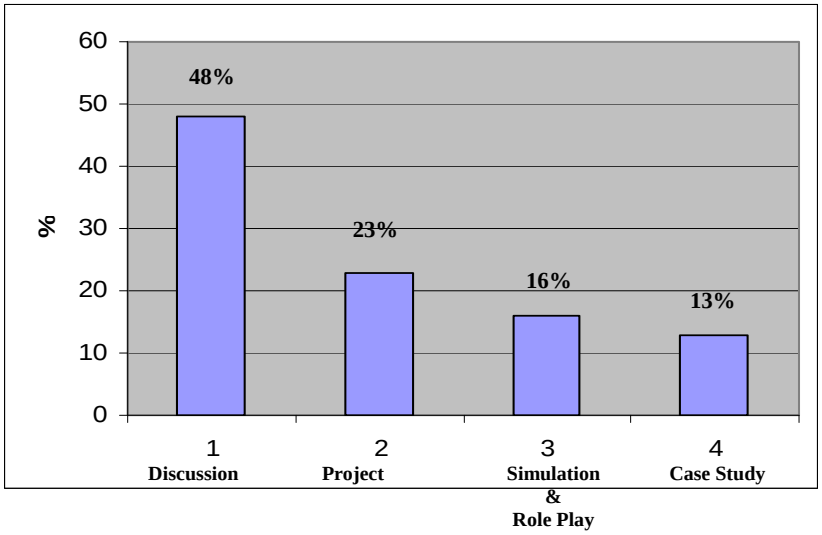

Figure 4. Teaching technologies priorities

As the bar graph shows, the students have given their preferences to activities which bear characteristics of communicative interactions, both spoken and written, which contribute to their ability to communicate in English. 48% of students give their adherence to discussion. 23% like working in groups and prefer Projects. 16% are attracted by simulations and role plays, especially shy students, since they become more talkative when playing roles and do not have to take responsibility for their own actions and words – in other words, it is the character they are playing who speaks, not themselves. 13% mentioned case study. In a less formal study I asked the students what they think about using Cases in the learning process. Most students confessed that they have too little idea about it as a teaching technology. It does not mean that teachers do not use Cases. We cannot avoid them today since most textbooks somehow deal with Case study. The problem might be that they are approached improperly. This might seem a bit frustrating since Project work and Case study are considered to be the leading contemporary technologies among the traditional arsenal of teachers not only in Europe but worldwide.

Communicative activities that the students have chosen mean getting them to actually do things with the language, and it is the '*doing*' that should form the main focus of the learning process.

6. Profile education model

Following the definition of profile education as well as research among students and having analysed all the collected data, our next task was to work out a model of profile education, which on the basis of general English at school level (Basic User level) will brush up the learners' previously acquired linguistic skills and will reinforce these with professional specialist knowledge and skills in different areas of their specialization to ensure an exit profile (Independent User level) and, ultimately, will take the students to a higher degree of proficiency in Business English, encouraging higher level language skills for professional needs (Proficient User level).

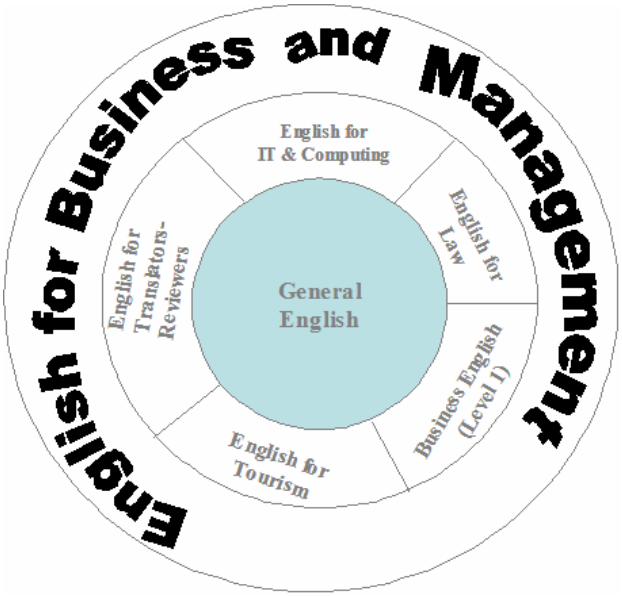

Figure 5. Profile education model

When one looks at the definitions of levels given in the description of the profile education model, one can see that they differ from the classic division into Basic, Intermediate and Advanced. Common Reference Levels are suggested by the Council of Europe in "Common European Framework of Reference: Learning, teaching, assessment" to help European partners 'to describe the levels of proficiency required by existing standards, tests and examinations in order to facilitate comparisons between different systems of qualifications and the public recognition of achievement.' [1]

Basic level corresponds to Level A – Basic User level (according to Council of Europe). Intermediate level corresponds to Level B – Independent User level. Advanced level corresponds to Level C – Proficient User level.

7. Project work and case study *(as the main elements of the syllabus structure)*

According to the Committee of Ministers of the Council of Europe, in the pursuit of the basic principles of successful language acquisition, 'we have to promote the national and international collaboration in the development of methods of teaching and evaluation in the field of modern language learning, to promote methods of modern language teaching which will strengthen independence of thought, judgment and action, combined with social skill and responsibility

- by basing language teaching and learning on the needs, motivations, characteristics and resources of learners;
- by defining worthwhile and realistic objectives as explicitly as possible;
- by developing appropriate methods and materials;
- by developing suitable forms and instruments for the evaluating of learning programs [1].

Giving our adherence to these principles, we resort to Project work and Case study as the main elements of our syllabus structure since these teaching technologies prove to be flexible, comprising traditional and progressive methods of teaching and corresponding to all the modern demands for the language learning since they promote:

- the development of the ability to use the English language for natural communication,
- learning of grammatical structures and lexical material in the context of different situations,
- practicing the use of language elements for realistic purposes,
- the development of students' general intellectual faculties,
- the acquisition of cognitive strategies and study skills,
- the development of different categories of thinking (e.g. research, logical, abstract, creative, reasonable, etc.),
- the development of students' cross-cultural awareness,
- the acquisition of problem solving skills,
- the acquisition of team job skills,
- developing presentation skills,
- mastering conferencing skills.

PROJECTS – longer, learner-centred pieces of work that involve research and presentation – are one of the ways of ensuring genuinely communicative uses of spoken and written English. The end-product is the most important thing here, and all the language use that takes place is directed towards the final version. [2]

Project work provides a natural framework for ***integrated skills activities.***

There is a tendency in language classroom to focus attention on one skill at a time: thus, in one lesson, or part of a lesson, special attention is paid to oral work; in another to reading and so on. Often, however, it is a pedagogical convenience rather than a necessity and probably reflects the way the skills have been sequenced in the unit of work in the course book: speaking/listening →reading→writing. This kind of sequencing reinforces language items, but does not integrative skills in any real sense.

Notice that in 'real life' we do not use language skills in any set order or in any necessary conjunction with each other. For example, if we read an interesting advertisement in the paper for a holiday, we may want to discuss it with our friend and then perhaps ring up or write for more information. This nexus of activities will involve reading→speaking/listening→either speaking /listening or writing, and may continue or stop at that point. It can provide a model for **integrating skills** in a realistic way. [8]

Of course, it cannot be suggested that single-skill activities are not effective: there will in fact be many occasions when we shall ask the students just to talk or read or write, because this is appropriate. Usually, however, we should be looking for opportunities to knit skills together, because this is what happens in real life. Project lesson helps to exceed the limits of the classroom, approaching, thus, the 'real world'.

It should be noted that projects cannot be fulfilled at once. At least three evident stages have to be passed through. Broadly speaking, we can distinguish three levels of tasks on our way to projects.

First level tasks aim basically at developing communicative abilities in a specific area of the language being taught. These tasks may include such activities as simulation, problem-solving, etc.

For example:

Simulation – is an activity where the learners discuss a problem (or perhaps a series of problems) within a defined setting. Let us look at a simple example to see what this involves. The students might be told:

A foreign business person is going to do business for the first time in your country. In his letter he is asking you for some advice about business practices in Latvia.

STUDENTS A: Prepare properly formulated questions about specific situations.
STUDENTS B: Use the appropriate structures to answer the questions on:

- Use of language: addressing/greeting (formal? Informal?)
- Non-verbal communication: handshaking, gestures and silence?
- Dress code in the office: formal? Informal?
- Socializing: attitudes: gift giving, eating, humour?
  Conversation topics: (religion? politics? salaries?)
- Business negotiations: punctuality/respecting the agenda?
  Negotiating styles: direct? indirect?
  When is the right moment for exchanging business cards?
  When is the right moment to mention money?

Second level tasks concentrate basically on content, language and procedure. The student is involved mentally in these fields and the tasks aim at developing not only language skills, but also general cognitive strategies of handling and organizing information. In a typical second level task we normally follow the pattern: analyse what information we need→decide on procedure→collect information→select relevant data→present material in an organized way→discuss and analyse process and results.

Language becomes an instrument for doing a 'real' piece of work. Language is then handled widely, globally, not sequentially. This implies using not some certain, but a wide range of lexical sets, structures and functions. An essential part of the activity is continuous processing of input (the language that students hear or read) and output (the language that the students have acquired) while reading for information, translating from the mother tongue, discussing, debating, producing reports, etc. Certain forms of topic-based and content-based learning as well as research-based project work belong to this category.

For example:

You have decided to open a fitness club at the Institute.

The objective of the task is to collect and analyse information on:

- finding a suitable place;
- bank services in Riga: giving loans, under what conditions;
- successful fitness clubs: kinds of equipment (photos, names of equipment);
- questionnaires: if a fitness club on demand, what kind of role you would like to perform (a visitor, a trainer);
- what kind of equipment is needed for your trainings.

1. Students decide:
   - what they need to know;
   - how to get this information (interviews, questionnaires, consultations with specialists);
   - where to get the information (banks, fitness clubs, library, the Internet, newspapers, magazines, etc.);
   - when to obtain the information;
   - what grids/database format they want to use to collate the information;
   - the kind of questionnaires/interviews they want to devise;
   - the language they need to carry out the interviews.
2. Students carry out the research, transcribe the information obtained from consultations and interviews and put it together.
3. Students select relevant data, decide on a format (posters, beamer slides, dossier, etc.).
4. Students make a report and present it.
5. Students analyse the quality of the end-product, the process of creating it and the role of each participant in its creation (self-evaluation).

Third level tasks share the characteristics of second level tasks but have a wider scope. They involve all the aforementioned language and cognitive strategies and go a step further. They aim at developing the

personality of the student through the experience of learning a foreign language. Third level tasks fulfil wider educational objectives (attitudinal change and motivation, student awareness, etc.) and so are especially appropriate for the ordinary classroom conditions, where motivation for the learning of foreign language needs to be enhanced.

For example:

RURAL LATVIA IN MYTHS AND LEGENDS

1. Students and the instructor brainstorm aspects of the topic – places of interest in Latvia and some obscure or unknown spots in rural Latvia connected with national myths and legends.
2. Students are put into groups according to common interests. The groups identify the language and information they need.
3. The students carry out individual and group research on the selected topics. They discuss aspects of these 'obscure spots' and then report back.
4. The students decide on the different ways to link all research and present the final product (debates, reports, dramatization, slides, video, booklets translated in three languages, etc.).
5. Students present the topic and evaluate the activity.

There is some merit in the third level tasks, that is a high degree of task authenticity, globality, integration of language and contents, integration with other subjects and involvement of all the aspects of the individual's personality, previous experience and knowledge; this includes artistic, musical, literary interests, hobbies and concerns. Creativity is usually the factor that links all these elements.

So, summing up all the aforementioned we can say that *project work can be defined as a full implementation of a second or a third level task.* [8]

CASE STUDIES present realistic business situations and problems and communication activities based on them – group discussions, simulations and role plays – serve to enhance the authenticity of the course. A case study usually has several stages:

1. A particular situation is taken with an account of what happened to a business or industry over a number of years and describes the events and problems that managers had to deal with.
2. The instructor highlights the main aspects that have to be paid special attention and gives recommendations.
3. Learners study the situation, analyse it in groups and generate different ideas to find solutions to the problem. Then they draw up their suggestions for the presentation.
4. Presentation takes place where the solutions to the problem(s) are recommended.
5. A conference with the analysis of the quality of the recommendations and evaluation of everyone's contribution to these.

In our practice we have diversified the framework of case study. Taking into account that many of our students work part-time or combine work and studies during their final years at the Institute, we resort to home assignments in the form of cases. A student gets the task to visit his manager, to get him to know the methodology employed into the educational process and to find out the problems that the company is facing. Then he draws up the problem for the presentation in the class. So, in our case study we often begin with the presentation prepared by a student himself.

Such cases have proved to be much more engaging, since they are much closer to the students as they are touching their own interests. The problem is seen as very real and to solve it – it is the question of honour.

The purpose of the case study is to let students apply the concepts they have learned when they analyse the issues facing a particular company. To analyse a case study, therefore, they must examine closely the issues with which the company is confronted. Actually, they will need to read the case several times to grasp the overall picture of what is happening to the company and then several times more to get a clear understanding of the specific problems. [4]

Usually detailed analysis of a case study should include eight areas:

1. The history, development, and performance of the company over time.
2. The identification of the company's internal strengths and weaknesses.
3. The nature of the external environment surrounding the company.
4. A SWOT analysis.
5. The kind of corporate-level strategy pursued by the company.
6. The nature of the company's business-level strategy.
7. The company's structure and control systems and how they match its strategy.
8. Recommendations.

Cases prove valuable in a course for several reasons. First, cases provide students with experience of organizational problems that they probably have not had the opportunity to experience so far. In a relatively short period of time, they will have the chance to appreciate and analyse the problems faced by many different companies and to understand how managers tried to deal with them.

Second, cases illustrate what the students have learned. The theory and concepts help reveal what is going on in the companies studied and allow students to evaluate the solutions adopted by companies to deal with their problems. So, when analysing cases, a student will be like a detective who, with a set of conceptual tools, probes what happened and who was responsible and then marshals the evidence that provides the solution. Notice, that no one knows the right answer. In fact, managers say repeatedly that they are happy if they are right only every second time in solving strategic problems. Management is an uncertain game, and using cases to see how theory can be put into practice is one way of improving the skills of diagnostic investigation.

Third, case studies provide the opportunity to participate in class and to gain experience in presenting your ideas to others. Students learn to organize their views and conclusions so that they can present them to the class. Classmates may have analysed the issues differently and they will want to argue the points before accepting conclusions, so be prepared for debate. This is how decisions are made in the actual business world.

The individual or group probably will be responsible for the presentation of the case to the class. That presentation must cover the issues involved, the problems facing the company, and a series of recommendations for resolving the problems. Through class discussions and presentations, students will experience how to convey their ideas effectively to others, how to defend their ideas. It is important, that a great deal of manager's time is spent in these kind of situations, presenting their ideas and engaging in discussion with other managers, who have their own views about what is going on. Thus, students will experience in the classroom the actual process of what goes on in a business setting, and this will serve them well in their future career.

Working in groups students will learn about the group process involved in working as a team. There are always group members who shirk their responsibilities and group members who are so sure of their own ideas that they try to dominate the group's analysis. Most business negotiations take place in groups, however, and it is best if students learn about these problems now.

Case study, actually, imitates the mechanism of making decisions in real life, it is more adequate to live situations rather than learning terminology and then answering it to the teacher. The method demands not only the knowledge and understanding of certain terms but the ability to operate them as well, working out logical schemes of problem solving, giving reasons for the arguments and opinions. But the major merit of the method is the genuine interest of students towards it. Practice shows that they approach case study with immense enthusiasm and excitement, since the technology permits them to demonstrate their creativity, independence in judgements and at the same time demands demonstrating not only a spectrum of economical knowledge and skills but the ability to use these in practice. [4]

Since Project and case study give students full scope for working creatively and imaginatively for realistic purposes – learning through doing – and challenge their future professionalism, we find them fitting the curriculum goals.

The problem is that there is a great diversity of methods and techniques of teaching and learning English, but being taken in isolation they do not work and the results are still unsatisfactory. Therefore these impose the necessity to apply some integrative course comprising different fields of knowledge and touching different sides of life.

Project work and case study require some experimentation on the part of the teacher. Sometimes it is a slow process of trial and error. But, even when things do not go as expected, it is an exciting experience which teacher and students enjoy and learn a lot from, not only about language, but also about themselves and their own capacities.

8. Cognition process in the project work and case study

The interaction between student and teacher acquires a different style within the framework of projects and case study. They are no longer two opposite poles (i.e. the teacher renders information and the student perceives it) as in the more traditional type of teaching. Now they are two partners working together, planning, taking decisions, carrying out the task, and sharing the final sense of achievement. [8] The more so that now students learn not only from the sources of information, from the instructor, but also from each other. Within such a framework the instructor also gains knowledge, since students bring information into the classroom which does not relate exclusively to the linguistic area.

The process of cognition within the framework of projects and case studies can be presented in the diagram:

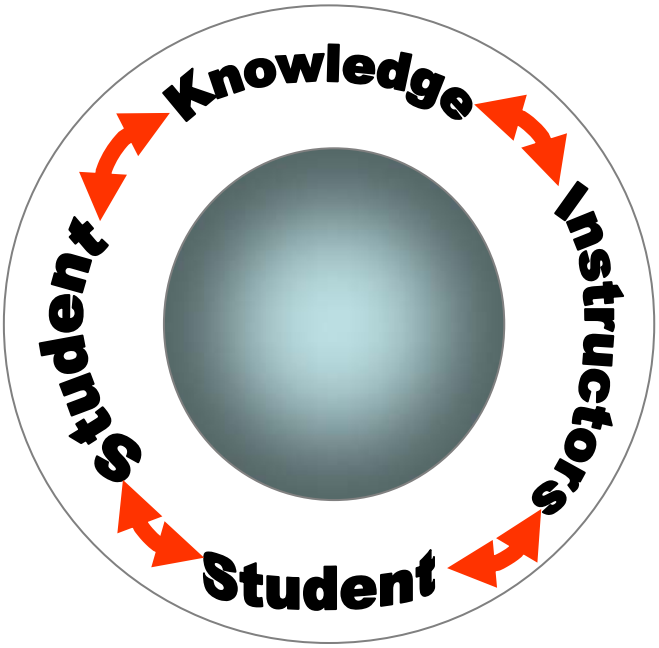

Figure 6. Cognition process in project work and case study

Teaching a foreign language, teachers often find it difficult to get all the students involved effectively into the process. To a large extent, it is because we are attempting *to teach in the classroom* what is normally – and perhaps best – *learned outside it.* The classroom is, of course, a convenient place for imparting information and for developing many educational skills, but our main concern as language teachers is not *to inform* our students *about the language* but to develop their ability *to use the language for a variety of communicative meaningful purposes.* That is why it is important to have a clear understanding and a firm grasp of the wide range of technologies and procedures through which oral ability can be developed. These technologies and procedures are *a way of accommodating language learning to the unfavourable environment of the classroom. Project work and case study help to solve this problem to a large extent.*

References

[1] *Common European Framework of Reference for Languages: Learning, teaching, assessment.* (2004) Cambridge University Press.
[2] Fried-Booth D. L. (2004) *Project Work.* Oxford University Press.
[3] Breen M., Littlejohn A. (2003) *Classroom Decision-Making.* Cambridge University Press.
[4] Nunan D. (2002) *Research Methods in Language Learning.* Cambridge University Press.
[5] Dudley-Evans T., Jo St. John M. (2002) *Developments in English for Specific Purposes.* Cambridge University Press.
[6] Harmer J. (2003) *The Practice of English Language Teaching.* Longman.
[7] Cotton D., Robbins S. (2003) *Business Class.* Longman.
[8] Ribe R. and Vidal N. (1993) *Project Work.* Heinemann.

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THEORETICAL DESCRIPTION OF OSCILLATING SURFACE REACTIONS: A COMPARISON OF MEAN FIELD, STOCHASTIC AND SIMULATION METHODS

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In this paper a kinetic model for the oscillating CO oxidation on reconstructing surfaces is studied by means of analytical and numerical methods at different levels of approximations. The methods are the mean field approximation neglecting all correlations, the cluster approximation taking into account only the correlations between nearest neighbours, and the correlation analysis, which considers all pair correlations, at least formally. The results are compared with simulation results. The model system exhibits kinetic oscillations in the reaction rate and the coverage of the surface species, which are closely connected with island formation and segregation. The consideration of long range and higher order correlations is of paramount importance for the correct description of systems with spatio-temporal structure formation.

As a consequence, only the correlation analysis is able to describe the system properties correctly in agreement with simulations, whereas the mean field and the cluster approximation fail to give correct results even at a qualitative level.

Keywords*: Computer simulations, Monte Carlo simulations, Models of non-linear phenomena, Models of surface chemical reactions*

1. Introduction

Surface reactions are of enormous importance for heterogeneous catalysis. Besides this practical importance one finds many complex and fascinating phenomena such as pattern formation and self-organization [1-3], regular and irregular oscillations [4-6], as well as chaotical behaviour [5, 7-9] even for apparently simple reactions over simple low index single crystal surfaces. A comprehensive review is given in ref. [10].

Although all these phenomena have been extensively investigated in the last 25 years the microscopic elementary reaction steps on an atomic length scale remain unclear. This problem can only be solved by *ab initio* calculations, but these methods will not be able to describe macroscopic systems and cooperative phenomena such as chemical waves and oscillations in the near future. Thus models based on stochastic methods are very much in demand. In such stochastic models very simple assumptions regarding the reaction mechanisms are made and often almost every detail about the reaction system is neglected (e.g. adsorbate-surface and adsorbate-adsorbate energetic interactions, geometric details and so on). Mainly two methods have been used in the recent past for the stochastic description of oscillations in surface reactions: (i) the mean field (MF) approximation or the so-called mathematical modelling (MM) and (ii) simulations based on Monte Carlo (MC) methods. Today, both types of theories exist for decades side by side and almost independent of each other.

The kinetic model for the oscillating CO oxidation used in the present paper has been studied in great detail and is able to explain several experimental facts, e.g. the origin of kinetical oscillations in the reaction rate as well as in the surface coverages [11, 12], the origin of and the relation between the non-linear growth rate and the critical adsorbate coverages [13] and the global synchronization of the oscillations [14, 15].

In this paper we do not want to study further properties of the model system. We study the model with mathematical methods at different approximation levels and compare the results of these. A similar study has been performed by Vigil and Willmore [16]. In this study they showed that the MF approximation "may not be appropriate when one or more species is strongly adsorbed" on the surface. Furthermore, they found that the pair mean-field approximation (PMF), which considers the influence of particle pairs on nearest neighbour sites, and the exact simulation of the system show only "small numerical discrepancies". They conclude that the reason for the applicability of the PMF approximation is that their model reaction involves only one-point and two-point processes. They expect that "greater disparity between the PMF and the lattics-gas simulation" might occur "for reaction mechanisms with processes involving three or more

neighbouring sites". We will show that this does not hold in general and that poor methods such as the MF approximation, the MM and the cluster or PMF approximation lead to wrong results even at a qualitative level for reaction systems with only one-point and two-point processes, i.e. these methods cannot give any physical insight to the reaction mechanism on the microscopic length scale. Therefore these should be seen as methods which can only be used to phenomenologically reproduce experimental results on the macroscopic length scale. This holds at least for models of surface reaction systems but should also generally hold for all systems showing spatial correlations. Of course there exceptions may exist in certain cases (e.g. refs. [14]). But the results of methods using approximation are not sufficient by themselves and always have to be compared with the exact results of lattice-gas simulations of the same system.

2. Model

We examine the oscillating $A + ½\ B_2 \rightarrow 0$ ($CO+O_2 \rightarrow CO_2$) reaction with the $\alpha \rightarrow \beta$ (*hex* $\rightarrow$1x1) structural transformation on a lattice. In our lattice gas model [11-14] we use a two-dimensional lattice with the lattice constant $a = 1$ and the coordination number z. In the work presented here we only deal with the regular square lattice ($z = 4$). Every lattice site can be covered with particle X with $X = 0$ (empty site), A or B. In addition the site itself can belong to the phase χ where χ stands for the α or β phase, respectively. This leads to a two parametric description X^{χ} and six different possible states for a single site on the lattice. E.g. A^{β} corresponds to a lattice site which is covered with a particle A and belongs to the β phase.

The adsorption of a particle A out of the gas phase is independent of the phase X the site belongs to. Therefore A adsorption is modelled in the same way as in the ZGB model [17] and the probability for A adsorption is given by the value of the gas phase mole fraction y.

It is known that the adsorption of B_2 dimers depends strongly on the phase of the lattice. On Pt(100), for example, the sticking coefficient for O_2 is about two orders of magnitude smaller on the *hex* phase than on the lxl phase. Corresponding to these experimental results [10] we model the dissociative B_2 adsorption as follows: One B_2 particle is adsorbed with probability $2(1 - y)$ if two empty nearest neighbour sites belonging to the β phase are found. Here $(1 - y)$ is the gas phase mole fraction of B_2. If at least one empty lattice site is in the α state B_2 cannot be adsorbed. Note that if the lattice is completely in the β phase the model coincides with the ZGB model [17].

It is known that CO is highly mobile on Pt(100) in the temperature range of the reaction and that the diffusion rates are several orders of magnitude larger than those of adsorption or desorption probabilities. Therefore the diffusion should be the most important reaction step in theoretical models for real surface reactions. The diffusion is modelled as a jump of an A particle into an empty nearest neighbour site. In first approximation we suppose that the phase of the sites plays no role for the diffusion process (see, however, refs. [13]). Our parameter D corresponds to the frequency factor for the diffusion (all transition rates in the stochastic theory are of dimension $[t]^{-1}$).

The AB reaction is simply an extension of the diffusion because now reaction occurs between A and B when a particle A jumps onto a site which is covered by B. When an A has jumped onto such a site the $A + B \rightarrow AB$ reaction takes place spontaneously and AB is removed from the surface. In our case the reaction is controlled by diffusion because reaction is a consequence of the motion of A particles.

The $\alpha \rightarrow \beta$ surface phase transition is modelled as a linear front propagation induced by the presence of CO in the border between phases with rate constant V. Consider two nearest neighbour surface sites in the state $\alpha\beta$. The transition $\alpha\beta \rightarrow \alpha\alpha$ ($\alpha\beta \rightarrow \beta\beta$) occurs if none (at least one) of these two sites is occupied by A.

The complete poisoning with A particles is possible and comes along with a macroscopic homogeneous β phase. Desorption of A from the lattice therefore should stabilize the surface structures in a way. Experimental results also indicate that A (CO) desorption is present at ambient reaction temperatures. We consider A desorption with rate constant k only in some cases of the MF and cluster approximation and mostly neglect it because even the model without A desorption shows oscillation phenomena.

3. Theoretical methods

The strongest simplification is the MF approximation. This theory neglects all spatial correlations in the system while it sets all pair correlation functions $F_{\lambda\mu}(\mathbf{r}) = 1$ ($\lambda, \mu = 0, A, B$) for all distances $\mathbf{r}$ [18]. This leads to a small set of coupled non-linear differential equations for the macroscopic densities. In the model presented here we get five independent bilinear equations.

The cluster approximation [18] considers only the correlations between NN pairs, i.e. $F_{\lambda\mu}(\mathbf{r}) = 1$ for $|\mathbf{r}| > 1$. The values of $F_{\lambda\mu}$ [1] may vary. With six macroscopic densities the cluster approximation gives 21 densities of pairs resulting in 20 independent non-linear equations with one additional normalization condition.

Although an increase in the number of equations is combined with the change from the simple MF approximation to the more complicated cluster approximation, both theories have the disadvantage that they cannot discriminate between microscopic and mesoscopic domains. If the model system exhibits the possibility of structure formation such as aggregation or segregation, these structures in a sense introduce a correlation length ξ, which characterizes the structure. Therefore the theory should be able to describe this correlation length. This is only possible if the pair correlation functions $F_{\lambda\mu}(\mathbf{r})$ are considered for every $r = |\mathbf{r}| > 1$, at least formally. The extension of the cluster approximation to obtain the correlation analysis [18] is similar to the extension of the MF approximation.

4. Results and discussion

In the present article we do not want to investigate in great depth the properties of the model but only want to show the variety of problems in modelling non-linear behaviour and pattern formation in surface reactions. We believe this is fundamental to understand theoretical tools and their applicability to treat phenomena in surface reactions (or systems exhibiting spatial correlations in general) on the microscopic length scale in order to get physical insight to the fundamental elementary processes.

For detailed studies on the influence of the individual parameters see refs. [11-14]. After having set up the system of MF equations one has to consider two points:

(1) Are the results of the MF approximation in qualitative agreement or at least comparable with the exact results of the simulation or with the results of the more precise approximations (cluster approximation or correlation analysis)?

(2) Are the equations of the MF approximation able to describe kinetic oscillations?

A good agreement with simulation results cannot be expected. An example is the original ZGB model [17] without any oscillations. In this model the simulation shows the existence of two phase transitions. For gas phase mole fractions of A, $y < y_1 = 0.387$ [19], the lattice is completely covered with B. With increasing y a second order (continuous) phase transition into a reactive state occurs until at $y = y_2 = 0.526$ [20] a first order (discontinuous) phase transition into an A poisoned state occurs. For $y > y_2$ the lattice is completely covered with A. The MF approximation confirms the existence of a first order phase transition ($y_{2,\mathrm{MF}} = 2/3$) but fails to give the correct result about the second order phase transition, which does not exist in the MF approximation for the ZGB model ($y_{1,\mathrm{MF}} = 0$). In this context it has to be stated, that the simulation result of the existence of the second order phase transition at y_1 is the exact result of the ZGB model, irrespective of the non-existence of such a transition in the real $CO+O_2$ surface reaction on Pt(100). The MF approximation gives incorrect results for the ZGB model which in turn gives incorrect results for the real $CO+O_2$ reaction on single crystal surfaces. Therefore the agreement of MF results with experimental results is only accidental and should not be seen as a correct result of a correct method to model surface reactions on atomic length scales. As a consequence one can expect large errors also for the MF description of kinetic oscillations because a transition from a steady state into an oscillating state can be seen as a kind of a phase transition.

All these errors of the simple MF approximation are connected to the complete omission of spatial correlations. The assumption of $F_{\lambda\mu}(\mathbf{r}) = 1$ for all $\mathbf{r}$ suggests that the different lattice states are distributed randomly (Poisson distribution) over the whole lattice. Of course, this is not the case. Let us consider some examples.

1) The investigation of the ZGB model shows that segregation phenomena exist, i.e. the A and B particles are not randomly distributed on the lattice but form more or less homogeneous islands of A and B, respectively. The $A + B$ reaction takes place only at the borders of the A and B islands. The MF approximation does not consider aggregation and segregation and the treatment remains incomplete or even worse, it is inconsistent. The reaction is over-emphasized in this approximation. For a detailed discussion see ref. [21].

2) The dissociative adsorption of B_2 takes place on a pair of vacant NN sites. These vacant lattice sites are created via the reaction of AB pairs on NN sites. Thus the vacant sites also show aggregation effects and the probability to find a vacant pair is larger than the product of the corresponding macroscopic densities. The MF approximation underestimates the dissociative B_2 adsorption.

3) Even worse for the model presented here is the assumption of randomly distributed surface phases. The MF treatment does not consider the distinction between mesoscopic and microscopic properties mentioned above, i.e. it is impossible to describe the formation of islands or any structures in general. Islands and length scales do not exist in the MF treatment.

The second question raised above deals with the description of oscillations. The description is possible in the framework of the so-called mathematical modelling. In this mathematical modelling the reaction system is described by a small number of coupled non-linear differential equations for the global densities. These equations are quasi-physical because most of the terms used can be derived directly from

the model using the MF approximation. On the other hand, some terms exist which cannot be explained by the model itself or derived from the MF treatment (e.g. precursor adsorption for CO [22], exponential growth rate for the nucleation of surface phases [23], non-linear dependence of the adsorption [24, 25]). These terms are introduced in a somewhat artificial way to create strong non-linearities in the corresponding equations because the possibility to find oscillating or otherwise complex solutions of a system of coupled non-linear equations strongly depends on the number of equations and their degree of non-linearity.

There exist two main differences between the MF theory and the mathematical modelling: (i) In the MF theory the number of equations and their structure is dictated by the reaction model. Their number changes only when more accurate approximations are used. (ii) The non-linearities should not be changed for any reason because they result ultimately from the law of mass action.

Therefore the mathematical modelling should be seen as an instrument to fit experimental results in order to describe the phenomenological kinetics. This is certainly justified and feasible but cannot at all be regarded as a microscopic model for surface reactions which aims at getting physical insight to the elementary reaction mechanisms on the microscopic length scale.

The simulation results are given in detail in refs. [11, 12]. The simulations have been performed with a very fast cellular automaton technique which agrees quantitatively with MC simulation results, at least for the oscillating systems considered here. Here we give a very concise summary to render possible the comparison of the simulation results with the results we discuss below. In the simulation the system shows a heterogeneous stable state with irregular oscillations which are locally synchronized by A diffusion. These oscillations exist for values of the A gas phase concentration $y < y' = y'(D,V)$, where y' is a critical point. The β phase builds small islands, which are dispersed in a macroscopic α phase. With increasing lattice side length L the various local oscillations are out of phase and effectively cancel each other. Therefore with increasing lattices the global oscillations have very small amplitudes. On very large lattices with $L \sim 10^7$, which would correspond to real surfaces but cannot be simulated today, these global oscillations should disappear. For $y > y'$ the system runs into a homogeneous absorbing state with $C_A = 1$ and phase coverage $\Theta_\beta = 1$.

The number of equations in the MF approximation is small enough to study the system quasi-analytically while searching for stationary solutions and examining their stability. In a second step the numerical analysis can be done.

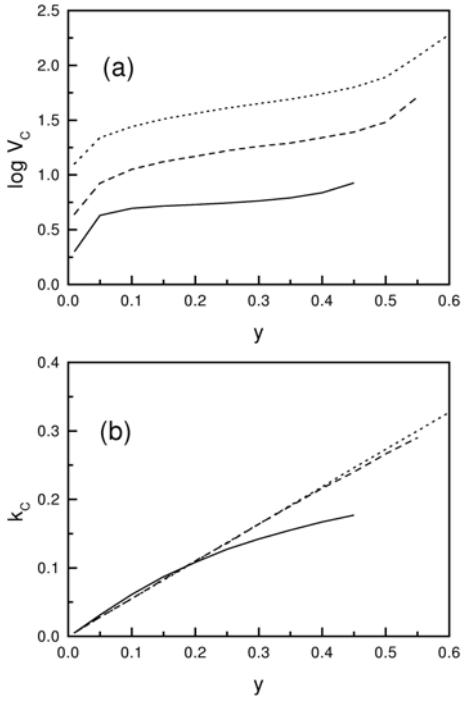

Figure 1. Critical values V_c and k_c in the MF approximation in dependence on the gas phase concentration of A for different values of the diffusion parameter (D = 10 solid line, D = 100 dashed line, and D = 1000 dotted line)

The stationary solutions of the non-linear system can be divided into two groups: (a) homogeneous solutions with $\Theta_\beta = 0$ or $\Theta_\beta = 1$ and (b) a heterogeneous solution with $0 < \Theta_\beta < 1$. If solution (b) exists, there is only one possible. At first we consider the minimal model with $k = 0$. In this case the poisoning of the surface with A is possible because desorption of A is neglected. Let ε_i be the eigenvalues of the stability matrix which corresponds to the temporal evolution exp ($\varepsilon_i t$) of the individual variables. The homogeneous solution $C_A = 1$ and $\Theta_\beta = 0$ is unstable. All values of ε_i are real except one value $\varepsilon_i > 0$. This instability results from the formation of the β phase because of the coverage by A. The solution $C_A = 1$ and $\Theta_\beta = 1$ is stable ($\varepsilon_i < 0$, attractor).

The main property of the heterogeneous solution is the mean value of the A coverage of about $C_A = 0.3$, i.e. it agrees almost quantitatively with the critical value C_A [13]. For the density of B $C_B < C_A$ holds with the limit of $C_B \to 0$ for $D \to \infty$. The value of Θ_β shows large variations. The heterogeneous solution exists in the domain $y < y^{(2)}$ with the critical value $y^{(2)} = y^{(2)}(D, V)$, e.g. $y^{(2)} = 0.582$ for $D = 100$ and $V = 1$. Here two complex eigenvalues ε_1 and ε_2 with $\varepsilon_{1,2} = p \pm i\omega$ exist. All other values ε_i are negative. p and ω depend on the parameters y, D, and V of the model. This solution can be unstable ($p > 0$) or stable ($p < 0$).

If we set $p = 0$ we can find the critical value $V_c = V_c(y,D)$ of the phase propagation constant V. The result is shown in Fig. 1(a). For $V < V_c$ ($V > V_c$) only unstable (stable) heterogeneous solutions exist with $p > 0$ ($p < 0$). In the following we restrict to values of V and D with $V << D$, although all values of V and D could be used. This is physically reasonable because the diffusion is the fastest process on surfaces, whereas the surface reconstruction is a slow many particle process which is connected with a significant mass transport and the rearrangement of the surface atoms. In most cases we use the constant value $V = 1$ and vary only the value of D. Thus stable heterogeneous solutions exist only for values of V which are too large to be physically reasonable [see Fig. 1(a)].

For small values of V the attractor ($C_A = 1$, $\Theta_\beta = 1$) should determine the system, but the number of the equations (five) is sufficient to give a more complex behaviour. The numerical investigation of the system of the kinetic equations shows a second critical point $y^{(1)} = y^{(1)}(D, V) < y^{(2)}$ which in addition is dependent on the initial conditions. Here we use the empty surface ($C_A = C_B = 0$) with a random distribution of the phases ($\Theta_\alpha = \Theta_\beta = 0.5$) as the standard initial condition. For $y > y^{(1)}$ the attractor drives the system into the absorbing (poisoned) state with $C_A = 1$ and $\Theta_\beta = 1$ This absorbing state is reached after a certain number of oscillations ($y < y^{(2)}$) or even without oscillations ($y > y^{(2)}$). For $y < y^{(1)}$ a limit cycle is reached which can be seen in Fig. 2, where the projection onto the three global variables of the five dimensional system is shown. For constant values of y and D the duration T of one period depends non-linearly on V.

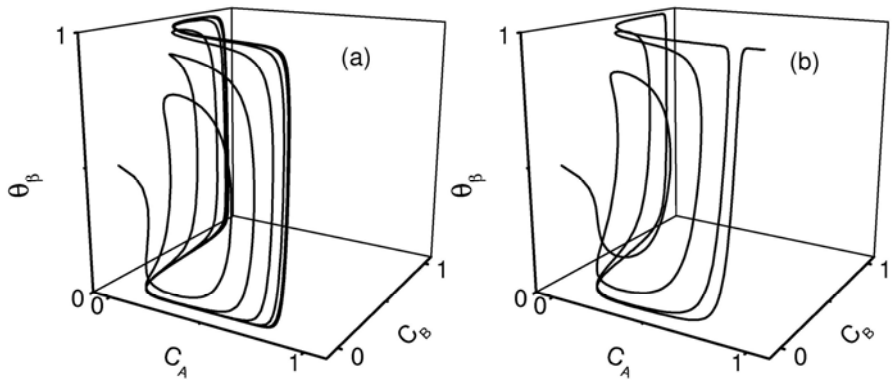

Figure 2. Transition from a limit cycle to an absorbing state in dependence on the A gas phase concentration y with D = 10 and V = 1: (a) y = 0.1, (b) y = 0.2

The *AB* production rate is not simply sinusoidal but shows non-trivial temporal structures which are given in Fig. 3. Although the solution of the equations shows a real periodic motion the resulting oscillations have a certain drawback. In the course of the reaction the β phase oscillates between $\delta < \Theta_\beta < 1 - \delta$ where $\delta = \delta(y, V, D)$ can become very small (of the order of 10^{-10}). Therefore it is inappropriate to regard these oscillations as real periodic motions of the heterogeneous system because on a finite surface these values of the phase would correspond to a transition into a homogeneous state. E.g. in a lattice gas simulation there would have to be at least $N > 1/\delta$ sites to show a heterogeneous state.

This problem can be solved by allowing A to desorb from the surface. With D and V constant the stability of the system ($p < 0$) strongly depends on the desorption probability k, for which a critical value $k_c = k_c(y, D, V)$ exists [see Fig. 1(b)]. For $k > k_c$ the system shows a stable heterogeneous state with δ not too small and of the order of $\delta > 0.05$. A second and trivial critical value can be obtained for k if the desorption probability becomes too large. In this case the system reaches a homogeneous α phase with $\Theta_\beta = 0$. Because k_c depends on y it is possible to get the following transitions if k, D, and V are kept constant. Starting with small values of y ($k > k_c$) one gets a stable heterogeneous state with oscillations. For medium values of y ($k \sim k_c$) a limit cycle is reached, whereas for large value of y ($k < k_c$) the system reaches an absorbing state. The expected heterogeneous stationary state without oscillations, which has been confirmed by simulations, is not obtained in the MF description of the model.

In the cluster approximation the number of equations is large and a quasi-analytical study is impossible. The results of a numerical treatment are qualitatively very similar to the MF approximation. This can be seen in Fig. 3(b) in comparison to part (a) in the same figure. For the same set of parameters

only small quantitative changes in the period and in the amplitude occur and the qualitative picture remains unchanged. In the cluster approximation the critical values $y^{(1)}$ and $y^{(2)}$ exist in agreement with the MF approximation. But in this case the attractor ($C_A = 1$, $\Theta_\beta = 1$) is much more effective because the value of $y^{(1)}$ is smaller than the corresponding critical value in the MF approximation. For values $y < y^{(1)}$ the heterogeneous state is stable even without A desorption, i.e. the value of $\delta = \delta(y, D, V)$ remains sufficiently large. This is clearly shown in Fig. 4(a). One systematic difference exists between the MF and the cluster approximation. As shown above the cluster approximation considers the correlation function between the nearest neighbours and its value may differ from unity.

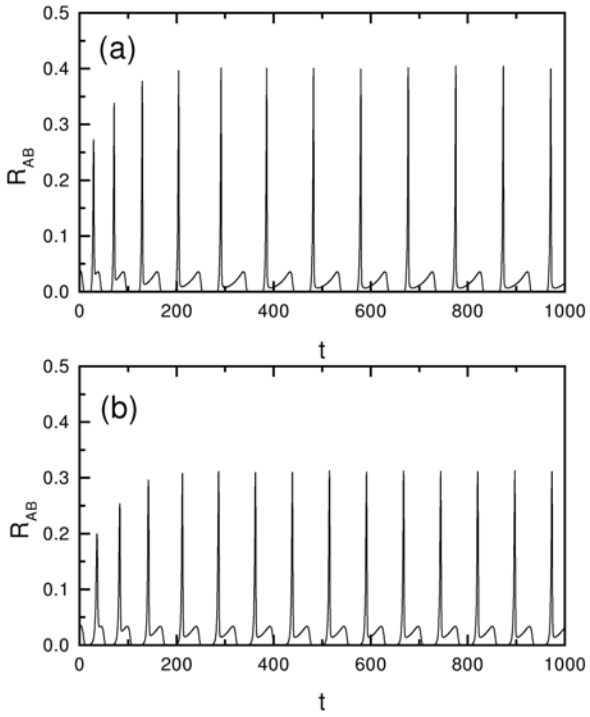

Figure 3. Temporal evolution of the AB reaction rate R_{AB} in the MF (a) and the cluster approximation (b) for y = 0.05, D = 10, and V = 1

This results in a temporal variation of the effective parameters such as the reaction "constant" K. In the MF approximation this reaction constant is a real constant and simply set to $K = D$. In the cluster approximation $K < D$ holds because the probability to find a reactive pair on NN sites is smaller than the corresponding product of the global concentrations. More important, the reaction "constant" K is not a constant anymore as soon as one considers correlations [21]. It is rather a variable with a temporal structure as shown in Fig. 4(b). This temporal structure is a consequence of the variation with time of the correlation functions, i.e. the effective reaction constant contains the structural alterations which take place in the course of the reaction.

The MF approximation and the cluster approximation are two methods which give very similar qualitative results. The reason for this is that both methods cannot describe structures and phenomena on a mesoscopic length scale such as aggregation and segregation.

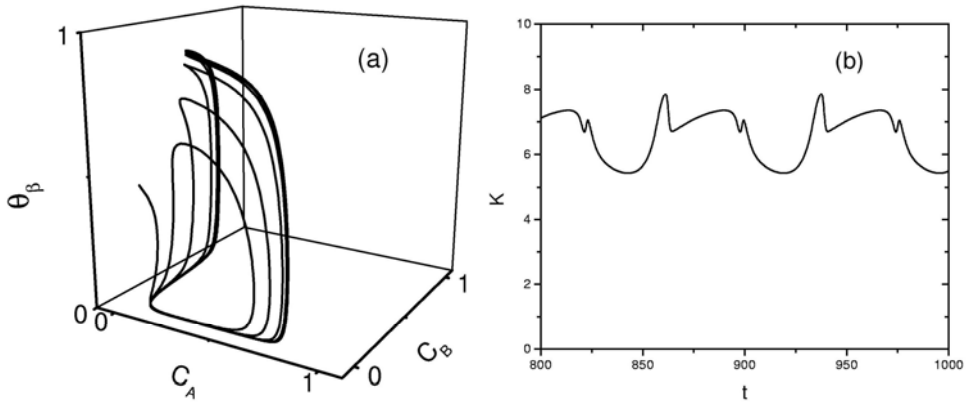

Figure 4. Limit cycle (a) and the effective reaction constant K (b) in the cluster approximation at y = 0.05, D = 10, and V = 1

But very often these phenomena have a large influence on the system properties. Again, a heterogeneously stable state without oscillations does not exist.

Formally the model should not show any oscillations in the limit of an infinite surface with a finite diffusion probability D because in this case it is impossible to globally synchronize the local oscillations.

This has been confirmed in a study by means of MC and CA simulations [11, 12]. Therefore the exact solution of the model should result in two different domains. For $y < y'$ a stable heterogeneous state should exist. In this interval the simulations give irregular oscillations which depend on the lattice size L. For $y > y'$, where the simulation reaches a poisoned state with $\Theta_\beta = 1$ and $C_A = 1$, a homogeneous stable state should exist with $\Theta_\beta = 1$. Because the correlation analysis can at least formally be applied to infinite systems ($L \rightarrow \infty$) in the thermodynamic limit it should be able to describe the above system properties. But the question about the synchronization is very complex. In the power spectra oscillations or traces of these are observed even in simulations on large lattices ($L \sim 10^3$) with moderate diffusion probabilities of $D = 100$. This means that long range spatial correlations of the order of L still exist between the adsorbate particles and between the surface phases even on such large lattices.

The correlation analysis considers only two point correlation functions $F_{\lambda\mu}(\mathbf{r}, t)$ and neglects all higher order correlations. This is certainly a drawback because in the case of such large spatio-temporal structures the correlations of higher order should play a certain role. In the numerical solution of the corresponding equations of the correlations analysis the equations are solved up to a maximum distance $r_{max}(t)$, where the correlation functions are different from unity and therefore non-trivial correlations exist. In all cases without desorption ($k = 0$) $r_{max}(t) < 10^3$ holds, i.e. in the correlation analysis lattices of side length $L = 1000$ of the corresponding simulation are sufficiently large (macroscopic), although they are of finite size.

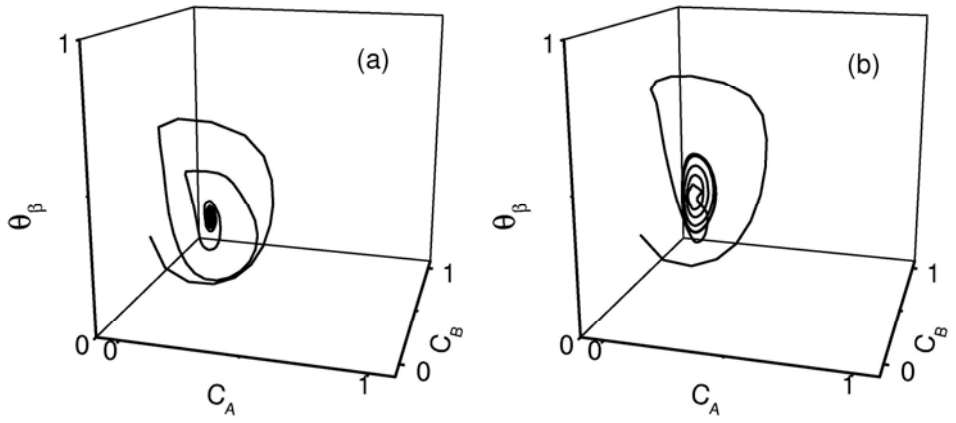

Figure 5. Relaxation into a stationary state (a) and the transition into a limit cycle (b) in the correlation analysis with y = 0.25 and y = 0.30, respectively. The other parameters are kept constant at D = 100 and V = 1

The correlation analysis shows certain deviations in comparison to the results above. Again two critical values resulting in three parameter ranges are obtained: For $y < y^{(1)}$ the system reaches a stable heterogeneous state without oscillations as shown in Fig. 5(a). This agrees with the above parameter range of $y < y'$. For $y^{(1)} < y < y^{(2)}$ the correlation analysis gives a transition into a limit cycle with small amplitudes as a result [see Fig. 5(b)]. This is a clear contradiction to the expected behaviour described above. In agreement with the theoretical expectations the system reaches a poisoned state for $y > y^{(2)}$.

Because the simulation results are the exact results of the model it is possible to compare these with the results of the correlation analysis. We compare the correlation analysis and the simulation for $y = 0.2 (y < y^{(1)})$, $D = 100$, and $V = 1$ on Fig. 6. After the initial relaxation the simulation shows very small oscillations for $t > 200$ but these are so small that we neglect them in the following. There exist two main differences between the two methods, (i) The oscillations in the correlation analysis are stronger damped than in the simulation. (ii) The density of B is larger in the correlation analysis as compared to the simulation. The other macroscopic variables (C_A, Θ_β, and R_{AB}) are in very good agreement between both methods. This shows that the model is very complex in a certain way. The B_2 molecules (the dimer) can only adsorb onto the β phase, which is highly dispersed, as can be seen in snapshots during the simulation [12]. These highly dispersed islands cannot be described correctly in the framework of the correlation analysis, which holds all the more for the MF approximation. This can also be seen in Fig. 7, where the results of the correlation analysis and the simulation are shown for $y = 0.3 (y^{(1)} < y < y^{(2)})$. Again the mean

values of the macroscopic variables are in very good agreement, with the exception of C_B. In addition to the relaxation time here also large deviations can be observed in the period of the oscillations.

The A desorption plays two roles in our model. On the one hand A desorption introduces a certain stability into the system. Although the considered desorption of A with $k = 0.1$ is weak the oscillations disappear and the macroscopic densities remain constant after some relaxation processes. The corresponding phase trajectories for different values of y are shown in Fig. 8. The system now shows the two theoretical solutions mentioned above, one leading to stationary heterogeneous states and one leading to a homogeneous state. But the stationary state is not a real stationary state. Although the macroscopic variables remain almost constant after relaxation, the pair correlation functions show spatio-temporal structure formation: spatial segregation of the different surface species. The correlation length $\xi(t)$ increases with time. The adsorbed B particles segregate into increasing islands, whereas the correlation function for adsorbed A remains almost constant at small values for different distances r. Also the surface phases show long range correlations and build islands of mesoscopic size. The correlation analysis shows qualitatively correct results with respect to the damped oscillations leading to a heterogeneously stable state without oscillations.

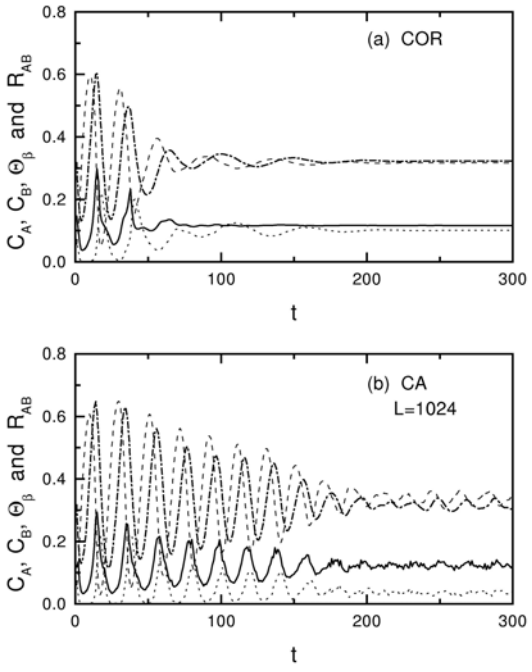

Figure 6. Temporal evolution of the surface concentration of A (dashed line) and B (dotted line), the coverage Θ_β (dot-dashed line) of the β phase and the AB production rate R_{AB} (solid line) for the correlation analysis (a) and the simulation (b). The parameters are y = 0.2, D = 100, and V = 1

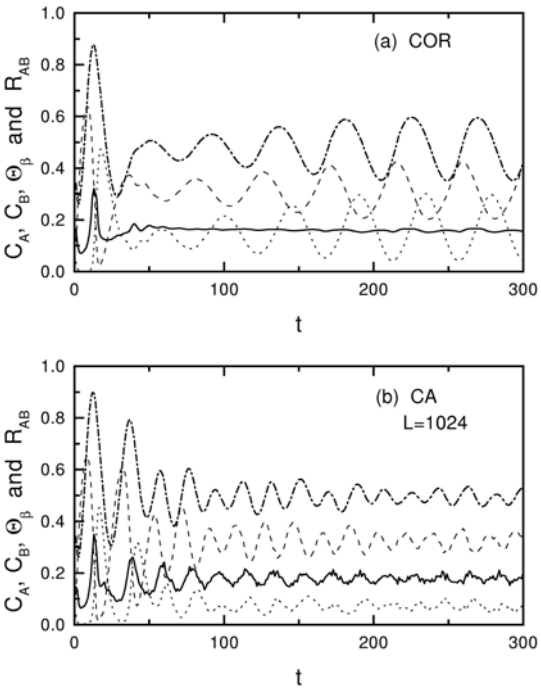

Figure 7. Temporal evolution of the surface concentration of A (dashed line) and B (dotted line), the coverage Θ_β (dot-dashed line) of the β phase and the AB production rate R_{AB} (solid line) for the correlation analysis (a) and the simulation (b). The parameters are y = 0.3, D = 100, and V = 1

5. Summary

In this paper we have studied a model for the heterogeneous $CO+O_2$ reaction on a surface with the $\alpha \rightarrow \beta$ reconstruction. In simulations [11, 12] the model exhibits a heterogeneous stable state for $y < y'(D,V)$ without any global, but only locally synchronized oscillations. The result of the correlation analysis agrees qualitatively with the simulation results. It shows a heterogeneous stable state with constant values for the global concentrations, i.e. without oscillations, as well as the transition into the homogeneous state for larger values of y. In a small parameter regime the correlation analysis leads to incorrect results. In this interval the solution exhibits limit cycle oscillations with small amplitudes and wrong frequencies compared to the simulation. The MF approximation and the cluster approximation lead to completely wrong properties of the system. The solution within these methods gives macroscopic (globally synchronized) limit cycle oscillations. These do not exist.

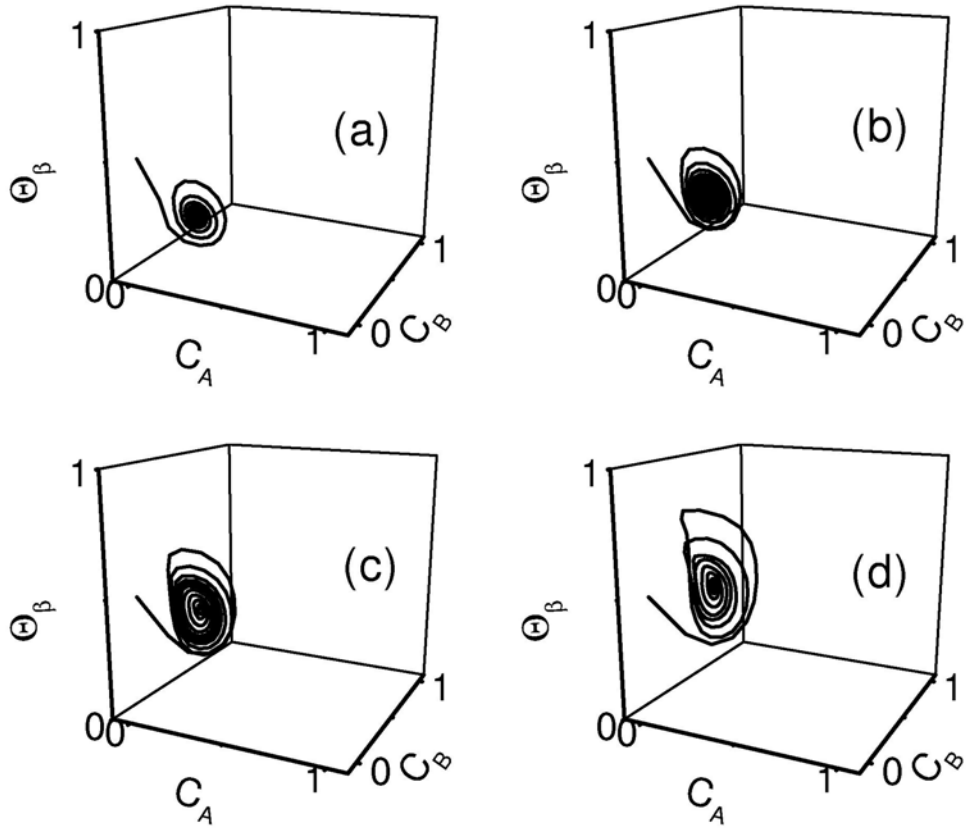

Figure 8. Relaxation into a stationary state in the correlation analysis with (a) y = 0.25, (b) y = 0.30, (c) y = 0.35, and (d) y = 0.40. The other parameters are kept constant at D = 100, V = 1, and k = 0.1

In almost every study on surface reactions in the literature the mathematical modelling has been used, i.e. the kinetic equations have not been derived from the model alone, but many additional assumptions and parameters have been introduced into the mathematical description of the corresponding systems. In general these parameters are additionally subjected to fitting procedures in order to get agreement with experimental results. In the context of our results and the complete failure of these mathematical methods to describe even our very simple model at least qualitatively correct it has to be doubted that any information about the underlying reaction mechanisms can be deduced from the mathematical modelling of surface reactions. This should also hold for all other systems which show spatio-temporal pattern formation and large long range correlations.

References

[1] Rotermund H. H., Engel W., Kordesch M. and Ertl G. (1990) Imaging of spatio-temporal pattern evolution during carbon monoxide oxidation on platinum. *Nature* **343,** 355-357.

[2] Jakubith S., Rotermund H. H., Engel W., von Oertzen A. and Ertl G. (1990) Spatiotemporal concentration patterns in a surface reaction: Propagating and standing waves, rotating spirals, and turbulence. *Phys. Rev. Lett*. **65**, 3013-3016.

[3] Veser G. and Imbihl R. (1992) Spatial pattern formation in the oscillatory NO+CO reaction on a Pt(100) surface and its vicinal orientations. *J. Chem. Phys*. **96,** 7155-7163.

[4] Veser G. and Imbihl R. (1994) Synchronization and spatiotemporal self-organization in the NO+CO reaction on Pt(100). I. Unsynchronized oscillations on the 1×1 substrate. *J. Chem. Phys*. **100,** 8483-8491.

[5] Veser G. and Imbihl R. (1994) Synchronization and spatiotemporal self-organization in the NO+CO reaction on Pt(100). II. Synchronized oscillations on the hex-substrate. *J. Chem. Phys.* **100**, 8492-8500.

[6] Fink Th., Dath J.-P., Imbihl R. and Ertl G. (1991) Kinetic oscillations in the NO + CO reaction on Pt(100): Experiments and mathematical modeling. *J. Chem. Phys*. **95**, 2109-2126.
[7] Veser G., Mertens F., Mikhailov A. S. and Imbihl R (1993) Global coupling in the presence of defects: Synchronization in an oscillatory surface reaction. *Phys. Rev. Lett*. **71**, 935-938.
[8] Eiswirth M., Kruel Th.-M., Ertl G. and Schneider F.W. (1992) Hyperchaos in a chemical reaction. *Chem. Phys. Lett*. **193**, 305-310.
[9] Cobden P. D., Siera J. and Nieuwenhuys B. E. (1992) Oscillatory reduction of nitric oxide with hydrogen over Pt(100). *J. Vac. Sci. Technol*. *A* **10**, 2487-2494.
[10] Imbihl R. and Ertl G. (1995) Oscillatory Kinetics in Heterogeneous Catalysis. *Chem. Rev*. **95**, 697-733.
[11] Kuzovkov V. N., Kortlüke O. and von Niessen W. (1998) Kinetic oscillations in the catalytic CO oxidation on Pt single crystal surfaces: Theory and simulation. *J. Chem. Phys*. **108**, 5571-5580.
[12] Kortlüke O., Kuzovkov V. N. and von Niessen W. (1999) Simulation of kinetic oscillations in surface reactions on reconstructing surfaces. *J. Chem. Phys*. **110**, 11523-11533.
[13] Kuzovkov V. N., Kortlüke O. and von Niessen W. (1999) Nucleation and island growth kinetics on reconstructing surface. *Phys. Rev. Lett*. **83**, 1636-1639.
[14] Kortlüke O., Kuzovkov V. N. and von Niessen W. (1999) Global synchronisation via homogeneous nucleation in oscillating surface reactions. *Phys. Rev. Lett*. **83**, 3089-3092.
[15] Salazar R., Jansen A. P. J. and Kuzovkov V. N. (2004) Synchronization of surface reactions via Turing-like structures. *Phys. Rev. E* **69**, 031604-1/4.
[16] Vigil R. D. and Willmore F. T. (1996) Oscillatory dynamics in a heterogeneous surface reaction: Breakdown of the mean-field approximation. *Phys. Rev. E* **54**, 1225-1231.
[17] Ziff R.M., Gulari E. and Barshad Z. (1986) Kinetic Phase Transitions in an Irreversible Surface-Reaction Model. *Phys.Rev.Lett*. **56**, 2553-2556.
[18] Mai J., Kuzovkov V. N. and von Niessen W. (1994) general stochastic model for the description of surface reaction systens. *Physica A* **203**, 298-315.
[19] Voigt C. A. and Ziff R. M. (1997) Epidemic analysis of the second-order transition in the Ziff-Gulari-Barshad surface-reaction model. *Phys. Rev. E* **56**, R6241-6244.
[20] Ziff R. M. and Brosilow B. (1992) Investigation of the first-order phase transition in the A-B_2 reaction model using a constant-coverage kinetic ensemble. *Phys. Rev. A* **46**, 4630-4633.
[21] Kotomin E. A. and Kuzovkov V. N. (1996) *Modern aspects of diffusion-controlled reactions: cooperative phenomena in bimolecular processes, Vol. 34 of Comprehensive chemical kinetics* / Edited by C. H. Bamford and R. G. Compton. Amsterdam: Elsevier.
[22] Imbihl R., Cox M. P., Ertl G., Müller H. and Brenig W. (1985) Kinetic oscillations in the catalytic CO oxidation on Pt(100): Theory. *J. Chem. Phys.* **83**, 1578-1587.
[23] Gruyters M., Ali T. and King D. A. (1995) Modelling temporal kinetic oscillations for CO oxidation on Pt/s(100/s). The (1×1)-CO island growth rate power law model. *Chem. Phys. Lett.* **232**, 1-6.
[24] Krischer K., Eiswirth M. and Ertl G. (1992) Oscillatory CO oxidation on Pt(110): Modeling of temporal self-organization. *J. Chem. Phys*. **96**, 9161-9172.
[25] Makeev A. G. and Nieuwenhuys B. E. (1998) Mathematical modeling of the NO + H_2/Pt(100) reaction: "Surface explosion," kinetic oscillations, and chaos. *Chem. Phys.* **108**, 3740-3749.

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CUMULATIVE INDEX

COMPUTER MODELLING and NEW TECHNOLOGIES, volume 10, No. 4, 2006

(Abstracts)

A. Gopeyenko, S. Piskunov, Yu. N. Shunin. The Atomic and Electronic Structure of Pure and Defective $PbZrO_3$, *Computer Modelling and New Technologies*, vol. 10, No 4, 2006, pp. 7-16.

First principles DFT (Density Functional Theory) calculations have been performed using hybrid exchange-correlation functionals B3PW and B3LYP containing an admixture of non-local Fock exchange. Calculated equilibrium geometry of orthorhombic (antiferroelectric) PZ is in a good agreement with the recent experimental observations. The influence of point defects to the ferroelectric nature of PZ is modelled by incorporating of single F^0-centre (oxygen vacancy containing two electrons) into the bulk crystal. The computed electronic structures for both pure and defective PZ are discussed.

Keywords: Density Functional Theory, F^0-centres

E. K. Shidlovskaya. Problem of Cluster Embedding in Crystalline Lattice, *Computer Modelling and New Technologies*, vol. 10, No 4, 2006, pp. 17-28.

General problem "subsystem in the field of the frozen remaining part of the whole electron system" is investigated in the framework of one-electron approximation. Orthogonality restrictions are not imposed on one-electron wave functions. Consideration is general for every task of this type (cluster and the rest of crystal, fragment of a molecule and the remaining part of it, valence and core electrons, etc.).

Total energy of the whole system (cluster + the rest of system) is expressed in terms of non-orthogonal one-electron wave functions. Equations for the cluster wave functions are obtained directly from variation of the total energy expression subject to the condition that wave functions of the rest of system are known and fixed. Mutual orthogonality constraints are not imposed during variation. Homogeneous equations resulting directly from general procedure are obtained first. Then they are transformed to the eigenvalue problem equations. Particular case of these equations giving mutually orthogonal one-electron wave functions of the cluster staying to be non-orthogonal to those of the remaining system is found. The remaining system wave functions are found not to be solutions of these equations.

Vacant solutions of the equations are studied. Initial equations are shown to have different structure for vacant and occupied cluster states. Initial equations are further modified in the way leading to the same structure for both occupied and vacant states and keeping occupied states unchanged.

Keywords: Quantum-chemical simulation, embedded molecular cluster model, non-orthogonal one-electron wave functions, localised molecular orbitals, theory of pseudopotentials

L. Kutsenko, D. Fuks, A. Kiv, M. Talianker, L. Burlaka, O. Monteiro, I. Brown. New Approach in *Ab initio* Description of Ion Beam Induced Phase Transformations, *Computer Modelling and New Technologies*, vol. 10, No 4, 2006, pp. 29-34.

Ab initio calculations are performed to study the phase transitions in Mg alloys induced by Plasma Immersion Ion Implantation (PIII). It was proposed a new approach for prediction of the formation of new phases based of the analysis of electronic characteristics of the intermediate state which is formed in the beginning of the ion induced phase transition. The mechanism of the formation of new structure Mg-28.35.at %.Al-18.34 at %Ag was found.

Keywords: phase transformations, ion implantation, Mg alloys

Yu-R. Kalninsh, G. Ozolinsh. Integrated Framework for Social, Economic or Business System Modelling, *Computer Modelling and New Technologies*, vol. 10, No 4, 2006, pp. 35-41.

This paper explores several possible advances in modelling dynamics of complex social, economic or business systems enabled by developments and standardization efforts driven by World

Wide Web Consortium and Object Management Group. In particular usage of Meta Object Facility and Semantic Web concepts in connection with system dynamics modelling technique is presented. Extension mechanism to support collaboration, standardization and reuse of system dynamics models and their applications is proposed.

Keywords: complex social, economic or business systems, computer modelling

R. I. Muhamedyev, E. Nikitina. Evaluation System of Risky Enterprises, *Computer Modelling and New Technologies*, vol. 10, No 4, 2006, pp. 42-45.

To differ risky enterprises the special system of evaluation is used now. Revenue office of the Republic of Latvia uses the system named "Eskort". The system must select enterprises that are potentially risky. Such enterprises are first candidates to audit. "Eskort" is a typically additive model of evaluation. The weakness of single level additive model of evaluation is considered in this report. This model is frequently used by test systems and other systems of evaluation. It is very simple but the single level additive model of evaluation cannot realize linear indivisible function. That is why the system for evaluation of risky enterprises cannot solve some problems. Some of them like XOR problem of one level neural network. Multi-layer neural nets and production systems described as the method of overcoming of drawbacks of additive model.

Keywords: neural nets, evaluation risky enterprises, production system

R. Tumasonis, R. Rastenis. New Statistical Characteristics for Mining Frequent Sequences in Large Databases, *Computer Modelling and New Technologies*, vol. 10, No 4, 2006, pp. 46-52.

The paper deals with the search and analysis of the subsequence in large volume sequences (texts, DNA sequences, etc.). A new algorithm ProMFS for mining frequent sequences is proposed and investigated. It is based on the estimated probabilistic-statistical characteristics of the appearance of elements of the sequence and their order. The algorithm builds a new much shorter sequence and makes decisions on the main sequence in accordance with the results of analysis of the shorter one.

Keywords: Data Mining, frequent sequences

A. Baublys. The Econometric Models of Forecasting of the Transport Flows, *Computer Modelling and New Technologies*, vol. 10, No 4, 2006, pp. 53-60.

The importance of forecasting the economic characteristics of transportation (i.e. the amount of freight and passengers carried, the turnover rate of freight and passengers, etc. in transportation as a whole and in particular areas using various transport facilities) is demonstrated. Methods for predicting the development of transportation based on multidimensional regression and correlation analysis and realizing mathematical models for finding linear and non-linear multidimensional regression equations as well as a mathematical model for choosing linear and non-linear regression equations, more accurately approximating the empirical data, are presented.

The techniques aimed to obtain and apply the linear correlation coefficient and correlative relationship in determining the forecast accuracy is also given. The efficiency of methods, determining the linear correlation coefficient and correlative relationship, used in achieving higher accuracy of forecasts is shown.

Keywords: forecasting, multidimensional regression, correlative analysis, mathematical models, approximation, empirical data, correlative relationship, linear correlation coefficient

N. I. Volkov, A. N. Kochevsky, S. V. Sapozhnikov. Distance Learning for Specialities Belonging to Mechanical Engineering, *Computer Modelling and New Technologies*, vol. 10, No 4, 2006, pp. 61-65.

The paper presents experience of activity of Sumy State University aimed at preparation and implementation of distance learning for specialities belonging to mechanical engineering, development of corresponding learning and methodical materials, description of technical and organizational aspects of this activity. The paper presents also the authors' vision concerning future development of modern forms of education of specialists of technical profile.

Keywords: distance learning, mechanical engineering

A. Mishenin. Using Counter Propagation Neural Network for Building Intellectual Decision Support Systems, *Computer Modelling and New Technologies*, vol. 10, No 4, 2006, pp. 66-69.

Commonly, complex modern manufactures systems' controlling makes its operators pass important decisions what sometimes is rather difficult when there are many alternatives. Such situation requires developing and involving of automatic intellectual decision support systems (DSS). Different approaches have been already developed in order to help operator with passing correct decisions. Each has its advantages and disadvantages.

This work presents a new approach to building decision support systems based on modified counter propagation neural network. Intellectual self-training automatic control systems and intellectual self-training decision support systems allow switching from old subjective methods of manual control to up to date intellectual informational control technologies for badly formalized processes and objects functioning under uncertain conditions. The following main tasks of the presented work have arisen from this assertion.

Keywords: automatic intellectual decision support systems

T. Lobanova. Teaching Techniques in Profile Education, *Computer Modelling and New Technologies*, vol. 10, No 4, 2006, pp. 70-79.

The specifications for profile education reflect the objectives of the Information Systems Management Institute curriculum presented in the "Common European Framework of Reference for Languages: Learning, teaching, assessment", issued by the Educational Committee of the Council for Cultural Co-operation in 2004 and in the 'Standards for Modern Foreign Languages' issued by Latvian Ministry of Education and Science in 1998.

The curriculum defines what language learners have to learn in order to use the language for communication and what knowledge and skills they have to develop so as to be able to act effectively in different domains.

It is very important for the specialists working in the field of modern languages to provide a common basis for the objectives, content and methods applied, to overcome the barriers to communication arising from the different educational systems in Europe, and to enhance the transparency of courses and syllabuses which will facilitate the mutual recognition of qualifications gained in different learning contexts [1].

Keywords: profile education, competences, communicative language competences, domain, case study, project work

V. N. Kuzovkov, W. Von Niessen, O. Kortlüke. Theoretical Description of Oscillating Surface Reactions: A Comparison of Mean Field, Stochastic and Simulation Methods, *Computer Modelling and New Technologies*, vol. 10, No 4, 2006, pp. 80-89.

In this paper a kinetic model for the oscillating CO oxidation on reconstructing surfaces is studied by means of analytical and numerical methods at different levels of approximations. The methods are the mean field approximation neglecting all correlations, the cluster approximation taking into account only the correlations between nearest neighbours, and the correlation analysis, which considers all pair correlations, at least formally. The results are compared with simulation results. The model system exhibits kinetic oscillations in the reaction rate and the coverage of the surface species, which are closely connected with island formation and segregation. The consideration of long range and higher order correlations is of paramount importance for the correct description of systems with spatio-temporal structure formation.

As a consequence, only the correlation analysis is able to describe the system properties correctly in agreement with simulations, whereas the mean field and the cluster approximation fail to give correct results even at a qualitative level.

Keywords: Computer simulations, Monte Carlo simulations, Models of non-linear phenomena, Models of surface chemical reactions

COMPUTER MODELLING and NEW TECHNOLOGIES, 10.sējums, Nr.4, 2006

(Anotācijas)

A. Gopeyenko, S. Piskunov, Yu.N. Shunin. Tīrā un defektīvā $PbZrO_3$ atomu un elektroniskā struktūra, *Computer Modelling and New Technologies,* 10.sēj., Nr.4, 2006, 7.-16. lpp.

Pirmie DFT aprēķinu principi ir veikti, pielietojot hibrīda apmaiņas-korelācijas funkcionāļus B3PW un B3LYP, kas satur nelokālo Foka apmaiņas piemaisījumu. Aprēķinātā ortorombiskā (antiferroelektriskā) PZ *equilibrium* ģeometrija saskan ar iepriekšējiem eksperimentāliem novērojumiem. Punkta PZ ferroelektriskās dabas bojājuma ietekme tiek modelēta, apvienojot vienu vienīgu F^0*-centru* (skābekļa vakance, kas satur divus elektronus) kristāla masā. Rakstā tiek diskutētas aprēķinātās elektroniskās struktūras kā tīram, tā defektīvam PZ.

Atslēgvārdi: Blīvuma funkcionālā teorija (Density Functional Theory), F^0-centri

E. K. Shidlovskaya. Klastera ievietošanas problēma kristāliskajā režģī, *Computer Modelling and New Technologies,* 10.sēj., Nr.4, 2006, 17.-28. lpp.

Tiek pētīta vispārēja problēma „apakšsistēma visas elektronu sistēmas sasaldētās atlikušās daļas laukā" tuvinājuma struktūrā ar vienu elektronu. Ortogonalitātes ierobežojumi netiek piemēroti viļņa funkcijām ar vienu elektronu. Izpēte ir vispārēja katram šī tipa uzdevumam (klasters un kristāla atlikums, molekulas fragments un tā atlikusī daļa, valence un pamata elektroni u.c.).

Visas sistēmas kopējā enerģija (klasters + sistēmas atlikusī daļa) tiek izteikta neortogonālās viļņa funkcijas ar vienu elektronu terminos. Klastera viļņa funkciju vienādojumi tiek iegūti tieši no kopējās enerģijas izteiksmes subjekta variēšanas, kas pakļauts tam apstāklim, ka atlikušās sistēmas daļas viļņa funkcijas ir zināmas un fiksētas. Savstarpējās ortogonalitātes ierobežojumi netiek piemēroti variēšanas laikā. Vispirms tiek iegūti homogēnie vienādojumi, kas rodas tieši vispārējās procedūras rezultātā. Pēc tam tie tiek pārveidoti *eigenvalue* problēmas vienādojumos. Šo vienādojumu īpašais gadījums, kas dod iespēju savstarpējām ortogonālām klastera viļņa funkcijām ar vienu elektronu palikt neortogonālām pret atlikušās sistēmas viļņa funkcijām, kas arī tiek izskatīts pētījumā. Tiek parādīts, ka atlikušās sistēmas viļņa funkcijas nav šo vienādojumu atrisinājums.

Vienādojumu vakantie risinājumi tiek pētīti.

Atslēgvārdi: kvantu-ķīmiskā modelēšana, ievietotais molekulārais klasters, neortogonālas viļņa funkcijas ar vienu elektronu, pseidopotenciāļu teorija

L. Kutsenko, D. Fuks, A. Kiv, M. Talianker, L. Burlaka, O. Monteiro, I. Brown. Jauna pieeja jona stara fāzes pārveides izraisīšanas *Ab initio* aprakstā, *Computer Modelling and New Technologies,* 10.sēj., Nr.4, 2006, 29.-34. lpp.

Ab initio aprēķini tiek veikti, lai pētītu fāzes transformācijas Mg sakausējumos, ko rada Plasma Immersion Ion Implantation (PIII). Tika ierosināta jauna pieeja jaunu fāzu formēšanās paredzēšanai, kas pamatojas uz starpstāvokļa elektronisko raksturojumu analīzi, kurš tiek izveidots jonu izraisītās fāzes transformācijas sākumā. Tika atrasts jaunas struktūras izveides mehānisms Mg-28.35 at %. Al-18.34 at % Ag.

Atslēgvārdi: fāzes transformācijas, jonu implantēšana, Mg sakausējumi

Yu-R. Kalninsh, G. Ozolinsh. Integrētā struktūra sociālajām, ekonomiskajām un biznesa struktūrām, *Computer Modelling and New Technologies,* 10.sēj., Nr.4, 2006, 35.-41. lpp.

Autori šajā rakstā izpēta dažas iespējamās pieejas kompleksā, sociālā un biznesa sistēmu dinamikas modelēšanā, kas tiek sekmēts ar pilnveidošanos un standartizācijas sasniegumiem, ko realizē *World Wide Web Consortium* un *Object Management Group*. Autori rakstā izskata sevišķā *Meta Object Facility* un *Semantic Web* konceptu lietojumu saistībā ar dinamikas sistēmas modelēšanas tehniku. Šajā pētījumā tiek piedāvāts Izvēršanās mehānisms, lai atbalstītu sadarbību, standartizāciju un atkārtotu sistēmas lietošanu un tās pielietojumu.

Atslēgvārdi: kompleksā, sociālā un biznesa sistēma, datormodelēšana

R. I. Muhamedyev, E. Nikitina. Uzņēmumu ar riska pazīmēm novērtēšanas sistēma, *Computer Modelling and New Technologies,* 10.sēj., Nr.4, 2006, 42.-45. lpp.

Rakstā autori pievēršas jautājumam par novērtēšanas sistēmām, lai diferencētu dažādus riska uzņēmumus. Latvijas Republikas Valsts ieņēmumu dienests izmanto sistēmu, kas ir nosaukta par "Eskorts". Šīs sistēmas uzdevums ir atlasīt tos uzņēmumus, kuri ir potenciāli riskantie. Parasti šie uzņēmumi ir pirmie, kuros veic auditu. Sistēma "Eskorts" ir tipisks papildu novērtēšanas modelis. Raksta mērķis ir izskatīt šī modeļa vājākās vietas.

Atslēgvārdi: neironu tīkli, riska uzņēmumu novērtēšana, ražošanas sistēma

R. Tumasonis, R. Rastenis. Jauni statistiskie raksturojumi datizroces biežai secībai lielajās datu bāzēs, *Computer Modelling and New Technologies,* 10.sēj., Nr.4, 2006, 46.-52. lpp.

Rakstā ir parādīta apakšsecības analīze un pētījums liela apjoma secībās (tekstos, DNA secībās utt.). Tiek piedāvāts un izpētīts jauns ProMFS algoritms biežas secības datizrocei. Tas tiek pamatots uz secības elementu parādīšanās varbūtējiem statistiskiem raksturojumiem un to kārtību. Algoritms būvē jaunu daudz īsāku secību.

Atslēgvārdi: datizroce, biežas secības

A. Baublys. Transporta plūsmu prognozēšanas ekonometriskie modeļi, *Computer Modelling and New Technologies,* 10.sēj., Nr.4, 2006, 53.-60. lpp.

Rakstā tiek parādīts transportēšanas ekonomisko raksturojumu prognozēšanas svarīgums (i.e. pasažieru un kravas daudzuma pārvadājums, pasažieru un kravas apgrozījuma lielums etc.), lietojot dažādus transporta līdzekļus. Autors izstrādā metodes transportēšanas attīstības prognozēšanai, pamatojoties uz multidimensionālu regresiju un korelācijas analīzi un ņemot vērā matemātiskos modeļus lineāru un nelineāru multidimensionālu regresijas vienādojumu atrašanā, kā arī matemātisko modeli lineāru un nelineāru vienādojumu izvēlē, vēl precīzāk nosakot empīriskos datus.

Bez tam rakstā autors dod arī lineāro korelācijas koeficientu iegūšanas un lietošanas paņēmienus un korelatīvo saistību, nosakot prognozes precizitāti.

Atslēgvārdi: prognozēšana, multidimensionālā regresija, korelācijas analīze, matemātiskie modeļi, aproksimācija, empīriskie dati

N. I. Volkov, A. N. Kochevsky, S. V. Sapozhnikov. Tālmācība mašīnbūves specialitātēm, *Computer Modelling and New Technologies,* 10.sēj., Nr.4, 2006, 61.-65. lpp.

Autori rakstā parāda pieredzi, kas iegūta, strādājot universitātē. Autori izskata tālmācības sagatavošanu un ieviešanu specialitātēs, kas skar mašīnbūvniecību, apmācības pilnveidošanu un metodisko materiālu izstrādi, kā arī parāda tehniskos un organizatoriskos aspektus šajā jomā. Raksts parāda arī autoru vīziju, kas skar tālāko izglītības moderno formu pilnveidošanu tieši tehniskajās specialitātēs.

Atslēgvārdi: tālmācība, mašīnbūvniecība

A. Mishenin. Pretējās izplatīšanās neironu tīkla izmantošana lēmumu intelektuālās atbalsta sistēmas izveidei, *Computer Modelling and New Technologies,* 10.sēj., Nr.4, 2006, 66.-69. lpp.

Parasti mūsdienu sarežģītās vadības sistēmas izveidošana liek tā operatoriem pieņemt svarīgus lēmumus, kas bieži vien ir grūts uzdevums, jo pastāv daudzas alternatīvas. Šāda situācija prasa automātiskās intelektuālās lēmumu atbalsta sistēmas pilnveidošanu un iesaistīšanu. Pašlaik jau ir izstrādātas dažādas pieejas, lai palīdzētu operatoram pieņemt pareizos lēmumus. Protams, katrs no tiem ietver kā plusus, tā mīnusus.

Šis konkrētais darbs piedāvā jaunu pieeju lēmumu atbalsta sistēmas izveidē, kas pamatota uz izmainīto pretējās izplatīšanās neironu tīklu.

Atslēgvārdi: automātiskās intelektuālās lēmumu atbalsta sistēmas – *angl.* automatic intellectual decision support systems

T. Lobanova. Apmācības metodes profila izglītībā, *Computer Modelling and New Technologies,* 10.sēj., Nr.4, 2006, 70.-79. lpp.

Profilās izglītības specifikācijas parāda Informācijas sistēmu vadības institūta mācību programmas uzdevumus, kas savukārt iekļauts dokumentā – „Common European Framework of Reference for

Languages: Learning, teaching, assessment", ko ir izdevusi Kultūras sadarbības padomes Izglītības komiteja 2004. gadā, kā arī Latvijas izglītības un zinātnes ministrijas 1998. gadā sagatavotajā materiālā – „Mūsdienu svešvalodu standarts".

Mācību programma norāda, kādu valodu apgūt, lai to varētu lietot komunicējot, un kādas zināšanas un prasmes ir jāpilnveido, lai efektīvi darbotos dažādās vidēs.

Atslēgvārdi: profilā izglītība, kompetences, komunikatīvās valodas kompetences, vide, projekta darbs

V. N. Kuzovkov, W. von Niessen, O. Kortlüke. Oscilējošās virsmas reakciju teorētiskais apraksts: vidējā lauka salīdzinājums, stohastiskās un modelēšanas metodes, *Computer Modelling and New Technologies,* 10.sēj., Nr.4, 2006, 80.-89. lpp.

Šajā rakstā tiek izpētīts kinētisks modelis oscilējošā CO oksidācijai uz rekonstruētām virsmām ar analītisko un skaitlisko metožu palīdzību dažādos aproksimācijas līmeņos. Metodes ir vidējā lauka aproksimācija, neievērojot nevienu korelāciju, klasteru aproksimāciju, ņemot vērā tikai korelācijas starp tuvākajiem kaimiņiem un korelācijas analīzi, kas apskata visas pāru korelācijas, vismaz formāli. Iegūtie rezultāti tiek salīdzināti ar modelēšanas rezultātiem.

Rezultātā rakstā tiek secināts, ka tikai korelācijas analīze ir spējīga aprakstīt korekti sistēmas īpašības saskaņā ar simulācijām, savukārt vidējais lauks un klasteru aproksimācijas nespēj dot pareizus rezultātus pat kvalitatīvajā līmenī.

Atslēgvārdi: datora simulācijas, Monte Carlo simulācijas, nelineārā fenomena modeļi, virsmas ķīmiskās reakcijas modeļi

COMPUTER MODELLING & NEW TECHNOLOGIES

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Computer Modelling & New Technologies * Preparation of publication

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The journal is being published since 1996.

PREPARATION OF CAMERA-READY TYPESCRIPT: COMPUTER MODELLING AND NEW TECHNOLOGIES

A Guide for Authors

A.N. AUTHOR
Affiliation
Institute address

Abstract reviews the main results and peculiarities of a contribution. Abstract is presented always in English or in English and the second (presentation) language both.
Keywords: main terms, concepts

1. Introduction

These instructions are intended to provide guidance to authors when preparing camera-ready submissions to a volume in the **CM&NT**. Please read these general instructions carefully before beginning the final preparation of your camera-ready typescript.

Two ways of preparing camera-ready copy are possible:
(a) preparation on a computer using a word processing package;
(b) printed copy fitted for scanning.

2. Printer Quality, Typing Area and Fonts

IMPORTANT:

If you produce your camera-ready copy using a laser printer, use a 15 x 23 cm typing area (in A4 format: 30 mm – left, 30 mm – right, 30 mm – top, 30 – bottom, line spacing – single), as in these instructions, in combination with the **10 points Times** font. The pages will then be reproduced one to one in printing.

Fonts

The names and sizes of fonts are often not the same on every computer system. In these instructions the Times font in the sizes 10 points for the text and 8 points for tables and figure legends are used. The references section should be in the 10 points font.

3. Format and Style

The text should be in clear, concise English (or other declared language). Please be consistent in punctuation, abbreviations, spelling (***British English***), headings and the style of referencing.

Camera-ready copy will be printed exactly as it has been submitted, so please make sure that the text is proofread with care.

In general, if you prepare your typescript on a computer using a word processing package, use styles for the font(s), margin settings, headings, etc., rather than inserting these layout codes every time they are needed. This way, you will obtain maximum consistency in layout. Changes in the layout can be made by changing relevant style(s).

4. Layout of the Opening Page

A sample for the opening page of a contribution is shown in Figure 1 on page 3.

Requirements for the opening page of a contribution are (see also Figure 1): the titles should always be a centered page and should consist of: the title in capital letters, bold font, flush center, on the fourth text line; followed by the subtitle (if present) in italics, flush center, with one line of white above. The author's name(s) in capitals and the affiliation in italics should be centered and should have two lines of white space above and three below, followed by the opening text, the first heading or the abstract.

5. Headings

Please distinguish the following four levels of headings:

1. First-order Heading

This heading is in bold, upper and lowercase letters, numbered in Arabic figures, and has two lines of space above and one line below. The text begins full out at the left margin.

1.1. SECOND-ORDER HEADING IN CAPITALS

This heading is in roman capitals, numbered in Arabic figures and has one line of space above and below. The text begins full out at the left margin.

1.1.1. *Third-order Heading in Italics*

This heading is in italics, upper and lower case letters, numbered in Arabic figures and has one line of space above and no space below. The text begins full out at the left margin.

Fourth-order Heading in Italics. This heading is in italics, upper and lowercase letters, with one line of space above the heading. The heading has a full stop at the end and the text runs on the same line.

↕ 3 blank lines

TITLE OF CONTRIBUTION

Subtitle of Contribution

↕ 2 blank lines

A.N. AUTHOR

Affiliation

Institute address

↕ 3 blank lines

Abstract

↕ 2 blank lines

First text line

Figure l. Example of an opening part of contribution to a Volume of CM&NT

6. Figures and Photographs

- *Line drawings* must be submitted in original form, on good quality tracing paper, or as a glossy photographic print.
- *Halftone photographs* must be supplied as glossy prints.
- *Colour illustrations.* Colour illustrations are more expensive and the author is expected to cover the extra costs. Please consult with Editors about this.

Mount all illustrations directly into the text at the appropriate places. Alternatively, it is acceptable to leave the appropriate space blank in the text, and submit the illustrations separately. In this case You must put the figure numbers in pencil in the open spaces in the text and on the back of the figures. Also indicate the top of the illustration.

For computer plotting the ORIGIN Software is preferable.

- Legends for figures/illustrations should not be incorporated in the figure itself and they should be listed in numerical order (headed as "*Figure 1.*", "*Figure 2.*" etc.). The legends should be set centered, below the figure.

7. Displayed Equations

Displayed equations should be in the left side of the page, with the equation number in parentheses, flush right.

$$E_{int} = \iint \psi^{+}(\mathbf{x})\psi(\mathbf{x})K(\mathbf{x}-\mathbf{x}')(-div\mathbf{P}(\mathbf{x}'))d^3x d^3x', \quad (1)$$

$$K(\mathbf{x}-\mathbf{x}') = C_0 \frac{exp(-\lambda(|\mathbf{x}-\mathbf{x}'|)}{|\mathbf{x}-\mathbf{x}'|}. \quad (2)$$

Font sizes for equations are: 12pt – full, 7pt – subscripts/superscripts, 5pt – sub-subscripts/superscripts, 18pt – symbols, 12pt – subsymbols.

8. Tables

Please center tables on the page, unless it is necessary to use the full page width. Exceptionally large tables may be placed landscape (90^0 rotated) on the page, with the top of the table at the left-hand margin. An example of a table is given below:

TABLE 1. National programs of fusion research [1]

Experiment	Type	Laboratory	Task	Begin of operation
JET	tokamak	Joint European Torus, Culham, UK	Plasma physics studies in the region close to ignition	1983
TEXTOR	tokamak	FA, Jülich. Germany	Studies of plasma-wall interaction	1982
TORE SUPRA	tokamak	CEA, Cadarache, France	Testing of super-conducting coils, stationary operation	1988
ASDEX Upgrade	tokamak	IPP, Garching, Germany	Plasma boundary studies in divertor plasmas	1990
WENDELSTEIN 7-AS	stellarator	IPP, Garching, Germany	Testing the principles of ”advanced stellarator”	1988
WENDELSTEIN 7-X	stellarator	IPP, Greifswald, Germany	Testing feasibility of ”advanced stellarator” for power station	2004

9. References

The References should be typeset in a separate section as a numbered list at the end of your contribution in the following style:

Journal articles should consist of as follows: author's name, initials, year, title of article, journal title, volume number, inclusive page numbers, e.g.:

[1] Dumbrajs O. (1998) Nuclear Fusion. *RAU Scientific Reports & Computer Modelling & New Technologies* **2,** aa-zz

[2] Kiv A.E., Polozovskaya I.A., Tavalika L.D. and Holmes S. (1998) Some problems of operator-machine interaction. *RAU Scientific Reports & Computer Modelling & New Technologies* **2**, aa-zz

[3] Shunin Yu.N. (1996) Elementary excitations and radiation defects in solids induced by swift heavy ions. *RAU Scientific Reports & Solid State Electronics & Technologies* **1**, 15-35

[4] Schwartz K. (1996) Excitons and radiation damage in alkali halides. *RAU Scientific Reports & Solid State & Electronics & Technologies* **1**, 3-14

Book references should consist of as follows: author's name, initials, year, title of book, publisher, place of publication, e.g.:

[5] Schwartz K. (1993) The Physics of Optical Recording. Springer-Verlag, Berlin Heidelberg New York
[6] Shunin Yu.N. and Schwartz K.K. (1997) Correlation between electronic structure and atomic configurations in disordered solids. In: R.C. Tennyson and A.E. Kiv (eds.). Computer Modelling of Electronic and Atomic Processes in Solids. Kluwer Academic Publishers, Dordrecht, pp. 241-257.

Unpublished papers should consist of as follows: author's name, initials, year (or: in press), title of paper, report, thesis, etc., other relevant details, e.g.:

[7] Shunin Yu.N. (1995) Elementary Excitations in amorphous solids accompanying the swift heavy ions passages. Private communication. GSI Seminar. Darmstadt

The references above should be cross-referenced by numbers within square brackets:
...as cited in [1], or Kiv *et al.* [2]... The use of author's initials for cross-references is not encouraged.

10. Authors Index

Editors form the author's index of a whole Volume. Thus, all contributors are expected to present personal colour photos with the short information on the education, scientific titles and activities.

11. Submission

Check your typescript very carefully before it is submitted. Submit two copies of the typescript to the Editors of the Volume. Always retain a copy of all material submitted as backup.

11.1. DISK FORMATS AND WORD PROCESSING PACKAGES

If you want to present contributions electronically please before submitting accord with the Editors the details on your computer system, your word processing package and version (MS Word 6 and above versions are preferable) and the way of transfer on the information (disk or Internet).

Acknowledgements

Acknowledgements (if present) mention some specialists, grants and foundations connected with the presented paper. The first page of the contribution should start on page 1 (right-hand, upper, without computer page numbering). Please paginate the contributions, in the order in which they are to be published. Use simple pencil only.

TSI

The K. Kordonsky Charitable Foundation

The 7th International Conference

RELIABILITY and STATISTICS in TRANSPORTATION and COMMUNICATION (RelStat'07)

24-27 October 2007. Riga, Latvia

PURPOSE

The purpose of the conference is to bring together academics and professionals from all over the world to discuss the themes of the conference:

- Theory and Applications of Reliability and Statistics
- Reliability and Safety of Transport Systems
- Rare Events and Risk Management
- Modelling and Simulation
- Intelligent Transport Systems
- Transport Logistics
- Education Programmes and Academic Research in Reliability and Statistics

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English and Russian will be the official languages of the Conference.

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DEADLINES AND REQUIREMENTS

Submission of abstracts:	**15 May**	**2007**
Acceptance of abstracts:	**29 May**	**2007**
Submission of final papers:	**3 July**	**2007**
Acceptance of final papers:	**4 September**	**2007**

Abstracts (about 600 words in length) and papers submitted for review should be in English and, should present a clear and concise view of the motivation of the subject, give an outline, and include information on all authors (the full name, affiliation, address, telephone number, fax number, and e-mail address of the corresponding author).

Submitted abstracts and papers will be reviewed. Accepted and invited papers will be published in the proceedings of the conference and in the journal "Transport and Telecommunication" (ISSN 1407-6160).

Instruction for papers preparing can be found on the conference WWW page: http://RelStat.tsi.lv.

INVITED SESSIONS (workshops)

Proposals for invited sessions (workshops) within the technical scope of the conference are accepted. Each proposal should describe the theme and scope of the proposed session. The proposal must contain the title and theme of the session and a list of paper titles, names and email addresses of the corresponding authors. Session proposals and paper must be submitted by **21 May 2007**.

REGISTRATION FEE

The registration fees will be **Euro 100** before 10 September 2006, and **Euro 150** after this date. This fee will cover the participation in the sessions, coffee breaks, daily launch, hard copy of the conference proceedings.

VENUE

Riga is the capital of the Republic of Latvia. Thanks to its geographical location, Riga has wonderful trade, cultural and tourist facilities. Whilst able to offer all the benefits of a modern city, Riga has preserved its historical charm. It's especially famous for its medieval part – Old Riga.

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A wide range of hotels will be at the disposal of participants of the conference and accompanying persons (http://eng.meeting.lv/hotels/latvia_hotels.php).

FURTHER INFORMATION

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