ISSN 1407-5806

COMPUTER MODELLING AND NEW TECHNOLOGIES

Volume 9
No 1

2005

Transporta un sakaru institūts
(Transport and Telecommunication Institute)

Computer Modelling and New Technologies

Volume 9, No.1 – 2005

ISSN 1407-5806
ISSN 1407-5814
(On-line: www.tsi.lv)

Riga – 2005

THE JOURNAL IS DESIGNED FOR PUBLISHING PAPERS CONCERNING THE FOLLOWING FIELDS OF RESEARCH:

- mathematical and computer modelling
- mathematical methods in natural and engineering sciences
- physical and technical sciences
- computer sciences and technologies
- semiconductor electronics and semiconductor technologies
- aviation and aerospace technologies
- electronics and telecommunication
- navigation and radar systems
- telematics and information technologies
- transport and logistics
- economics and management
- social sciences

Articles can be presented in journal in English (preferably), Russian, German and Latvian (at the option of authors). All articles are reviewed.

EDITORIAL CORRESPONDENCE
Transporta un sakaru institūts (Transport and Telecommunication Institute)
Lomonosova iela 1, LV-1019, Riga, Latvia. Phone: (+371)-7100593. Fax: (+371)-7100535.
E-mail: journal@tsi.lv, http:// www.tsi.lv

COMPUTER MODELLING AND NEW TECHNOLOGIES, 2005, Vol. 9, No.1
ISSN 1407-5806, **ISSN** 1407-5814 (on-line: www.tsi.lv)
Scientific and research journal of Transport and Telecommunication Institute (Riga, Latvia)
The journal is being published since 1996.

Computer Modelling and New Technologies, 2005, Volume 9, No.1

CONTENTS

Computer Modelling and New Technologies, 2005, Volume 9, No.1

Editors' Remarks

Of Many Worlds in this World

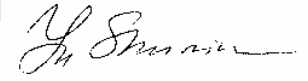
Just like as in a *Nest* of *Boxes* round,
Degrees of Sizes in each Box are found:
So, in this *World*, may many others be
Thinner and less, and less still by degree:
Although they are not subject to our *sense*,
A World may be no bigger than *Two-pence*.
NATURE is curious, and such Works may shape,
Which our dull *senses* easily escape:
For *Creatures*, small as *Atoms*, may be there,
If every one a *Creature's Figure* bear.
If *Atoms Four*, a *World* can make, then see
What several *Worlds* might in an *Ear-ring* be:
For, Millions of those *Atoms* may be in
The Head of one small, little, single *Pin*.
And if thus small, then *Ladies* may well wear
A *World of Worlds*, as *Pendents* in each *Ear*.

Margaret Cavendish[1]

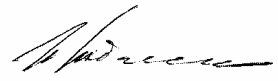
This 9th volume continues our main activities in solid-state physics, applied statistics, computer modelling, computer technologies and transport technologies. But new trends in science demand a special attention. In this respect, we must mention nanotechnologies. This field of science and technology will determine the society progress in all possible directions. The main reason is the principal evolution of information processing to the level of nano-sized objects. And we propose our authors to pay attention all possible aspects of nanotechnologies in their works. But this does not mean that the edition strategy is transformed essentially.

This edition is the continuation of our publishing activities. We hope our journal will be interesting for research community, and we are open for collaboration both in research and publishing.

EDITORS



Yu. N. Shunin



I.V. Kabashkin

[1] **Margaret Cavendish (1623-1673 -Duchess of Newcastle)** was an interesting character who had her first of many volumes of poetry published in 1653. In many ways contradictory in her work, she struggled between a desire for fame and the belief in the general benefit that education would give women. She is also known for her last published work, the life of her husband, William Newcastle, 1667, whom she met in 1645 after having accompanied Queen Henrietta Maria to France following the outbreak of civil war in England.

Computer Modelling and New Technologies, 2005, Vol.9, No.1, 7-14
Transport and Telecommunication Institute, Lomonosov 1, LV-1019, Riga, Latvia

AMPHOTERIC PROPERTIES OF Cr IN FeAl(B2) PHASE

A. STRUTZ, D. FUKS

Materials Engineering Department, Ben-Gurion University of the Negev,
P.O. Box 653, 84105 Beer Sheva, ISRAEL

The study of the influence of the vacancy on the Fe site and alloying by Cr on the band structure of the FeAl phase with the vacancy is performed on the basis of the Full Potential Augmented Plane-Wave (APW) + Local Orbitals (LO) method with WIEN 2k package. The changes in the total and the partial Densities of States (DOS), as a result of vacancy formation and alloying by Cr, are obtained and discussed. The formation of the "pocket" in the electron density in the vicinity of vacancy is revealed. We found that formation of the vacancy on the iron site leads to significant increase of the main peak in total DOS just below the Fermi energy together with the corresponding narrowing of the bands located below the Fermi level. The analysis shows that the formation of the vacancy on the Fe site leads to the creation of the damping wave of electronic excitations. Comparison of the partial DOS for d-electrons for different iron atoms in the extended cell clearly shows that this is the excitation of mainly d-states that reveal the same tendency as the total on-site DOS. At the same time the partial DOS for p-states for Al atoms does not show any noticeable change when the vacancy on the Fe site is formed. We found the changes in the site preference for Cr substituting for Fe or Al when the vacancy in FeAl(B2) phase is formed. The bonding tendencies and the changes in DOS in this case are discussed.

Keywords: *Fe-Cr, FeAl alloys, WIEN 2k package, Augmented Plane-Wave + Local Orbitals (APW+LO), Densities of States*

1. Introduction

Detailed information on the mass transfer in alloyed compounds demands the knowledge of vacancy formation and migration energies together with a clear understanding of diffusion mechanisms in these compounds. Nowadays a lot of investigations are focused on the study of these properties for intermetallics, and on FeAl in particular [1,2]. This is caused mainly due to versatile applications of these compounds in industry. The attention pointed on FeAl (B2) phase because of its low cost, low density, and resistance to corrosion and oxidation due to high aluminium content in this phase. These compounds have high concentration of point defects [3]. It is important to know how the ternary additives influence the characteristics of point defects in these compounds and what is the underlying physics that determines and controls the preferable site occupation for alloying elements in compounds with point defects. Recently, the investigation of the site preference of ternary alloying addition in FeAl (B2) phase by first principles calculations was performed [4] and a preference of Cr atom to occupy the position on the Al sublattice in FeAl (B2) phase was obtained. At the same time the existence of significant amount of vacancies may influence this preference because of the known amphoteric properties of Cr in Fe-Al.

The development of the theoretical study of vacancy-type defects (VTD) induced properties is limited by the necessity to consider solids with very low concentration of VTDs. The typical value of the VTD atomic fraction in d-metals is about 10^{-3} -10^{-5} and in semiconductors this value is even less ~10^{-8} - 10^{-10}. Thus the number of atoms that have to be taken into account in cluster or supercell calculations for metals should be 10^3 - 10^5. Nevertheless, the size of the supercell may be determined from the range over which VTD can effectively interact with each other. This is not directly related to the concentration of VTDs, which is a function of temperature and formation energy as they enter into Boltzmann balance equations. There should be some VTD-VTD separation distance beyond which VTD interactions are negligible and a relationship between vacancy formation energies and concentrations no longer exists. In this case the effective interaction radius, ρ_0, is the physical parameter, which determines the ability to receive VTD formation energy in the non-empirical calculations that is in agreement with the experimental data. The theoretical evidence of the existence of the physical parameter ρ_0 is proved by the calculations for Al [5], which shows almost no variation in the formation energy for the change of the supercell size from 8 to 32 atoms. These results indicate that this situation exists at quite high concentrations of vacancies in Al. Actually the VTD concentrations in this case are high and very far from reality but the obtained values are in a reasonable agreement with the measured data. For metals ρ_0 may be small due to the effective screening of the charge variations by the almost free electron gas.

The development of the density functional theory (DFT) [6,7] that is now included in numerous band structure techniques makes possible to obtain reliable results in large supercell modelling of different properties of alloys. Calculations of vacancy-dependent properties demand the accurate handling of supercell sizes and it leads to the necessity to use of the full-potential method. The program package WIEN2k [8] allows performing electronic structure calculations of solids using DFT. It is based on the Full Potential Augmented Plane-Wave (APW) + Local Orbitals (LO) method, one of the most accurate schemes for band structure calculations. In DFT the local (spin) density approximation (LSDA) or the improved version of the generalized gradient approximation (GGA) can be used as suggested in [9]. Both GGA and LSDA calculations are treated self – consistently and reproduce experimental value for lattice constant in impressive accuracy. In GGA not only the local density, but also its gradient determines exchange and correlation effects. However, it is shown in [10] that commonly used GGA functional fails to predict the experimentally stable DO_3 structure as the one with the lower total energy.

The variety of ground state properties of intermetallic compound FeAl with (B2) structure are investigated in recent research activities by the first principles calculations [11, 12] including the cohesive, electronic and magnetic properties [13]. Also a number of successful studies of vacancies in metals with WIEN2k package (see, for example, [14]) were performed.

In the present work, we report the results of the influence of the VTD on the Fe site and alloying by Cr on the band structure of the FeAl (B2) phase with the vacancy, using the self-consistent full-potential LAPW method. The changes in the total and the partial Densities of States (DOS), as a result of vacancy formation and alloying by Cr, are obtained and discussed.

2. Methodology

We have used the program package WIEN2k [8], which allows performing electronic structure calculations of solids, using DFT with the exchange-correlation functional in the form of a generalized gradient approximation (GGA). The GGA is the natural method of choice to describe a vacancy, since in this approximation the electron distribution shows large spatial variations. The Augmented Plane Wave with local orbital (APW+lo) method with spin polarization, as embodied in the WIEN2k code, was used to solve the Kohn-Sham equations. In APW+lo the unit cell is divided into two regions, in which two different types of basis sets are used: (1) inside atomic spheres, where electrons behave as they were in a free atom, a linear combination of radial functions times spherical harmonics is used; (2) an interstitial region between these atomic spheres, where the electrons are more or less 'free', a plane wave expansion is used. On the sphere boundary the wave functions of both regions are matched by value but their first derivative is discontinuous. The APW+lo basis set has proven to combine the LAPW ability of examine a large energy range with the smaller basis set size of APW. Thus, this version converges faster with respect to basis set and also reproduces all LAPW eigenvalues in an energy region around its linearization energy. The convergence of this basis set is controlled by the product $R_{mt}K_{max}$ between smallest atomic sphere radius in the unit cell, R_{mt}, and K_{max}, that defines the cut-off vector in reciprocal space. In order to improve convergence of basic set, we have to increase this product. A reasonably large R_{mt} can significantly reduce the computational time. In our calculations we choose a muffin tin radius R_{mt} =2.2 a.u and a plane–wave cut-off of $R_{mt}K_{max}$=9.

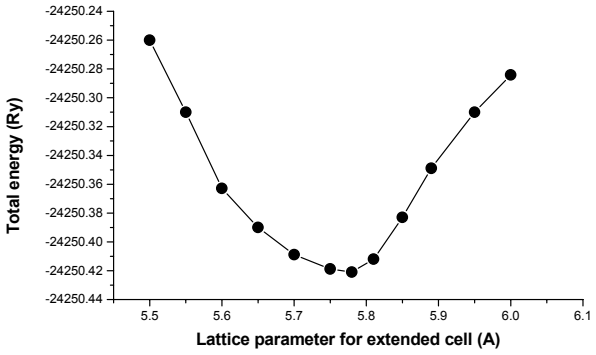


Figure 1. Dependence of the total energy on the lattice parameter for the $2\times2\times2$ extended cell in *FeAl (B2)* phase

The calculation of density of states (DOS) is employed by the modified tetrahedron method of Blöchl et al. [15]. We use the extended $2\times2\times2$ FeAl (B2) supercell in spin-polarized calculations. The accuracy of the total energy calculations was 10^{-4} Ryd.

3. Results and discussion

3.1. TOTAL ENERGY CALCULATIONS

The obtained value of the equilibrium lattice parameter is 5.78 Å for the extended cell (see Fig.1)

that is in excellent correlation with the experimental value 2.89 Å for the primitive B2 cell in FeAl [16] and with calculations of different groups [17,18].

In Table 1 we compare the results of our *ab initio* calculations for the primitive and the extended supercell in FeAl (B2) phase. The calculated formation enthalpies are in a good agreement with the experimental value.

TABLE 1. TOTAL ENERGIES FOR *Fe*, *Al*, *FeAl (B2)* PER CELL AND THE FORMATION ENTHALPY, ΔH_f FOR *FeAl (B2)* PHASE PER ATOM. ALL VALUES ARE IN Ry

Supercell	E_{Fe}	E_{Al}	E_{FeAl}	$\Delta H_{f,\,theor}$	$\Delta H_{f,\,exp}$[19]
1x1x1	-2545.61111	-485.6436	-3031.2843	0.0296	0.03829
2x2x2	-40725.7630	-7770.2976	-24250.4210	0.0428	

We have calculated also different characteristics for FeAl supercells with VTD on Fe site. The energy of vacancy formation, E_v and the volume formation, Ω_V, were defined as in [20]. For non-alloyed B2 phase E_v(FeAl)=0.787 eV that corresponds well to the experimental value E_v^{exp}=0.883 eV [21]. The calculated relative vacancy formation volume is 0.71.

To study the site preference of Cr in FeAl with and without the vacancy we performed a series of calculations. We analysed the total energies and the mixing energies for these cases according to the scheme suggested in [20]. The results are given in Table 2. It may be seen that the lowest mixing energy in FeAl with Cr in the case without the vacancy on the Fe site corresponds to the case when Cr substitutes for Al, although the difference in the mixing energies when this element substitutes for Fe or for Al is very small. This result is in agreement with *ab initio* calculations [4] and with the experimental data [22].

In the case, when the vacancy on the Fe site in FeAl is formed, the situation changes, and comparison of the mixing energies in this case shows that Cr prefers to substitute for Fe, as also may be seen from Table 2. The difference in the site preference occupation for Cr may be explained by comparison of the electro-negativity that is contributed by its nearest neighbours. When Cr substitutes for Al in the ideal FeAl phase his nearest neighbours are 8 Fe atoms and their electro-negativity contribution is 14.64 Pauling's. The vacancy formation on Fe site leads to the change in the site preference of Cr from the nearest neighbouring to the vacancy Al site to the second nearest neighbouring to the vacancy Fe site. In the case with VTD on Fe site, when Cr substitutes for Al, the number of his nearest neighbours changes to 7 atoms of Fe and their contribution of electro-negativity decreases to 12.81 Pauling's. This value is lower than the electro-negativity for the case when Cr substitutes for Fe site, that is 12.88 Pauling's, contributed by his nearest neighbours (8 Al atoms). At the same time, it worth to mention that the values of electro-negativity are rather close for different cases of substitution, that means that Cr does not have strong preference of Al or Fe sublattice. Nevertheless, comparing the mixing energy deviation for FeAl with VTD on Fe site and Cr shows more pronounced preference for Cr to occupy the Fe sublattice as compared with the case without VTD where Cr has only slight preference to occupy Al sublattice.

TABLE 2. THE TOTAL ENERGIES AND THE MIXING ENERGIES FOR *FeAl B2* PHASE ALLOYED WITH *Cr* WITH AND WITHOUT VACANCY ON *Fe* SITE FOR EXTENDED CELL $2\times2\times2$

	E_{mix} (Ry/atom)	E_{mix}^{vac} (Ry/atom)	E_{tot} (Ry)	E_{tot}^{vac} (Ry)
Cr on the Fe site	-0.0205	-0.0146	-23806.5292	-21260.8245
Cr on the Al site	-0.0214	-0.0127	-25866.5100	-23320.7603

We performed also the calculations of the energy of vacancy formation on Fe site when Cr occupies Fe or Al position near the Fe vacancy. When Cr substitutes for Fe that is the second nearest neighbour of the vacancy we found that the energy of the vacancy formation decreases in comparison with non-alloyed compound and for this case E_{vFe}(FeAlCr$_{Fe}$)=0.643 eV. When Cr substitutes for Al that is the first nearest neighbour of the vacancy the energy of the vacancy formation on the Fe site E_{vFe}(FeAlCr$_{Al}$)=0.949 eV. The energy of VTD formation on Fe site is much less when Cr occupies the Fe sublattice.

3.2. ANALYSIS OF THE DENSITY OF STATES

For the ideal FeAl (B2) phase the major contribution to DOS around Fermi energy, E_f comes from the narrow *d*-band of Fe *3d*-electrons. These states also form pseudo gap between the bonding and anti-bonding peaks. The contribution from *s*- and *p*-electrons of Al around E_f is negligible; they form relatively wide and flat bands.

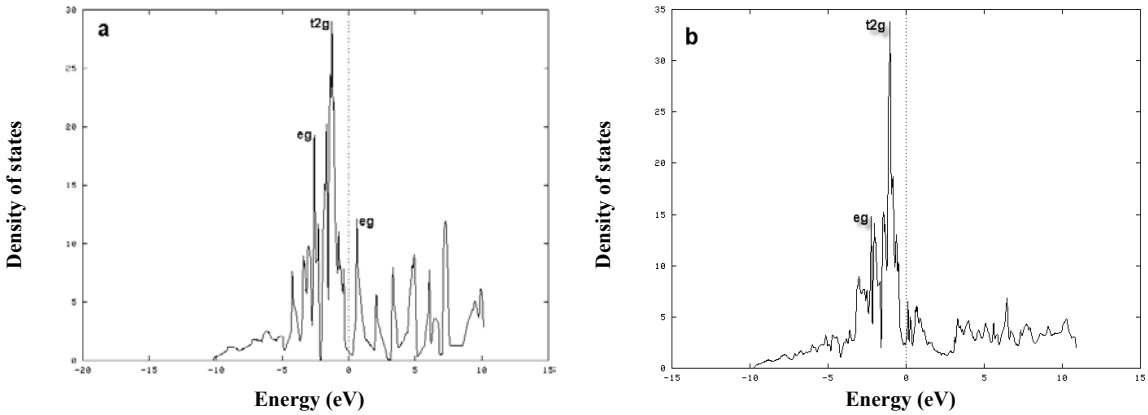


Figure 2. Total DOS for *FeAl B2* phase in extended $2\times2\times2$ supercell (a) without the vacancy and (b) with the vacancy on the *Fe* site.

We performed a detailed study of the influence of the VTD on the Fe site on the band structure of the (B2) phase. Figs. 2-3 very briefly illustrate the results of these calculations (we present here only spin-up DOS). Significant changes in the total density of states are found. Comparison of the DOS from Figs. 2-3 shows that formation of the vacancy on the Fe site leads to significant increase of the main peak that corresponds to t_{2g} *d*-electrons in total DOS just below the Fermi energy together with the corresponding narrowing of the bands located below the Fermi level. Our Fig. 3 demonstrates the changes of the on-site densities of states for different iron atoms that surround the vacancy on the Fe site (000) in the extended $2\times2\times2$ cell. The analysis shows that the main change occurs for the DOS for Fe atoms that are the first neighbours of the vacancy. We found a significant growth of the main peak in on site DOS for these atoms below the Fermi level. The DOS for the Fe atoms that are the second neighbours of the vacancy remains almost unchanged, while the DOS for the third neighbouring Fe atoms displays a slight growth of the main peak below the Fermi level as in the case for the first neighbours of the vacancy. It means that the formation of the vacancy on the Fe site leads to the creation of the damping wave of electronic excitations. Comparison of the partial DOS for *d*-electrons for different iron atoms in the extended cell shows that this is the excitation of mainly d-states that reveal the same tendency as the total on-site DOS. At the same time the partial DOS for *p*-states for Al atoms does not show any noticeable change when the vacancy on the Fe site is formed.

Studying the DOS for Cr in two cases (Fig. 4), when Cr substitutes for Fe in FeAl with the vacancy on the Fe site and when Cr substitutes for Al in ideal FeAl B2 phase we found a delicate interplay in the behaviour of electrons with spin up and spin down. For spin-up electrons the significant shift of mostly e_g- and less t_{2g}-states of Cr *d*-electrons to the low-energy region below the Fermi energy is observed. When Cr substitutes for Al in ideal FeAl these states of Cr *d*-electrons contribute to the conductivity of the material, while in the case when Cr substitutes for Fe in FeAl with the vacancy on the Fe site the well-defined minimum in the Cr DOS is observed in the vicinity of E_f. For spin-down electrons we observe the opposite but less pronounced behaviour. The total tendency is dictated thus by the spin-up electrons. The decrease of the conductivity in Cr-alloyed system with vacancy may be explained also as a consequence of the charge redistribution in this case and is linked to the higher localization of $d_{x^2-y^2}$-and d_{z^2}-electrons of Cr when this atom occupies the Fe site near the vacancy.

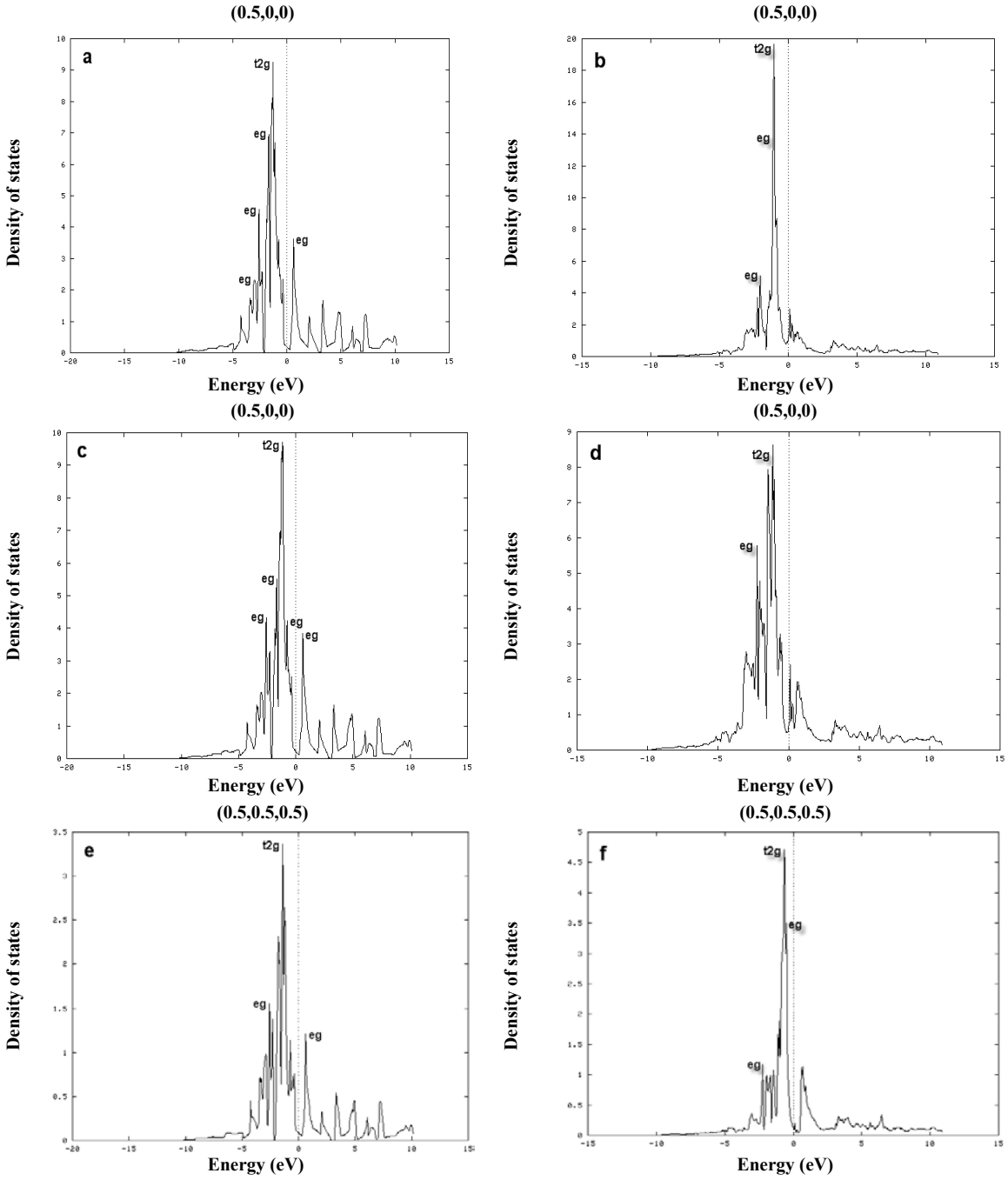


Figure 3. On site DOS for *Fe* atoms in the $2 \times 2 \times 2$ cell in *FeAl B2* phase with (b,d,f) and without (a,c,e) the vacancy on the *Fe* site in (000) position. The sites of corresponding *Fe* atoms are given in the graphs. All DOS are shown foe equilibrium lattice parameter that is 5.78 Å for the ideal cell and is 5.89 Å for the cell with the vacancy (only spin-up DOS is shown).

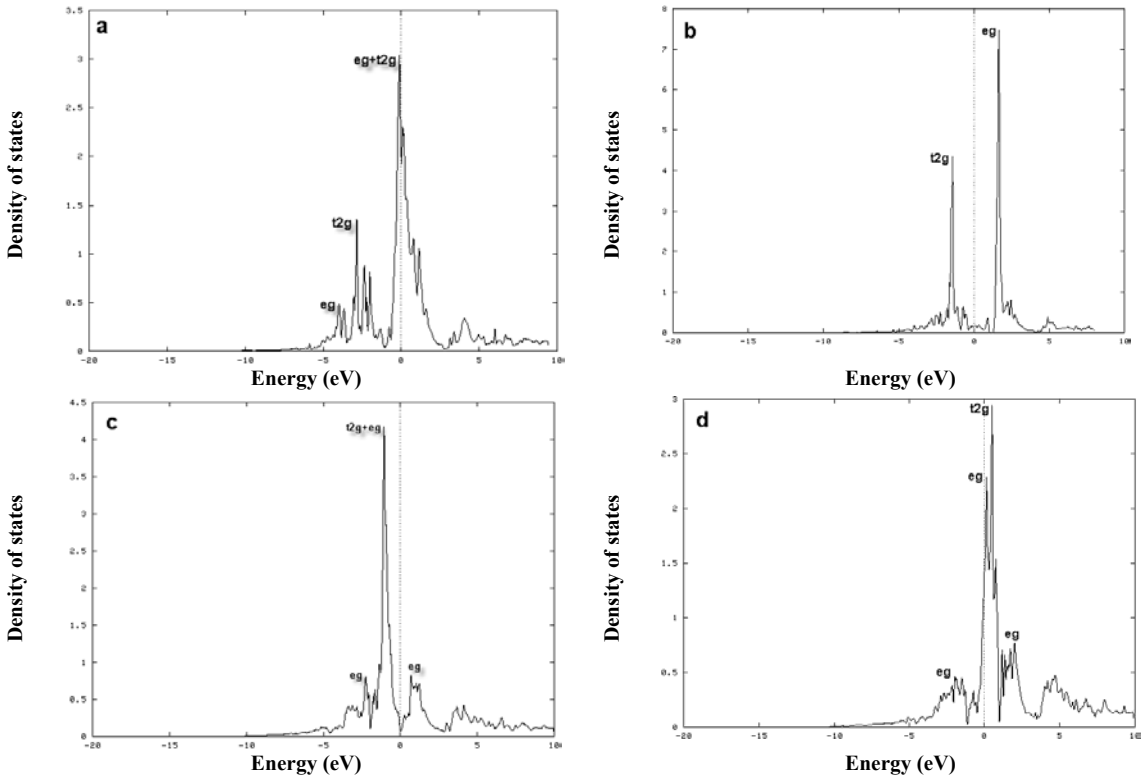
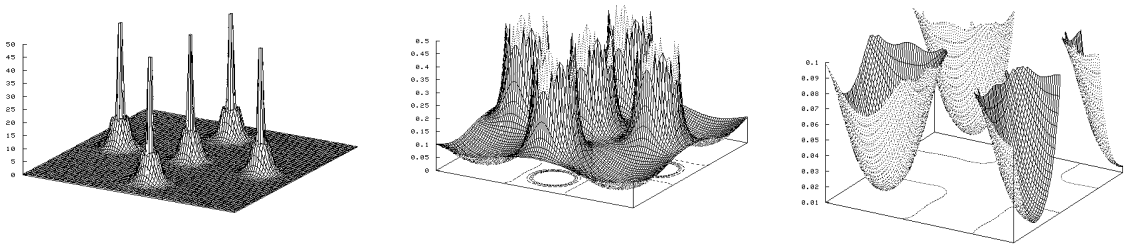


Figure 4. . On-site DOS for *Cr*: (a, c) spin up and (b, d) spin down for *FeAl B2* phase alloyed by *Cr* in extended $2\times2\times2$ super-cell. Cases (a, b) present the results without the vacancy and with *Cr* on *Al* site, (c, d) are the same with the vacancy and with *Cr* on *Fe* site.

3.3 CHARGE DISTRIBUTION

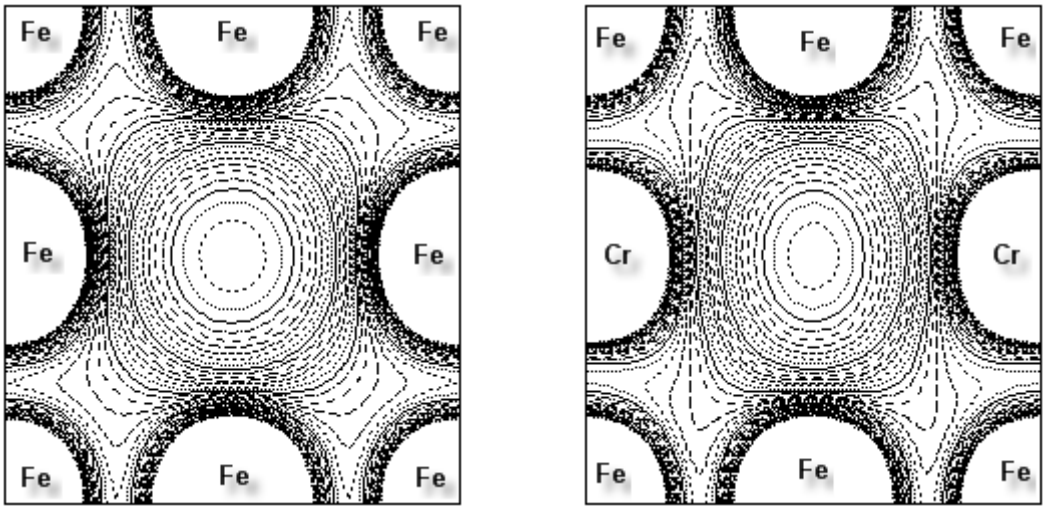
In Fig. 5 we show some of the results of our study of the charge redistribution in the vicinity of the vacancy formed on the Fe (000) site. It may be seen that the formation of the vacancy leads to creation of the "pockets" in the electronic density in the vicinity of the vacancy as in [23]. This means that the vacancy has some effective charge and may interact with each other.



a b c

Figure 5. (a) The cross-section of the electron density by the plane [100] in the extended cell of *FeAl (B2)* phase with the vacancy. (b) and (c) are the microscope view of the part from (a) that illustrate the topology of the electronic density in the vicinity of the vacancy.

To analyse the influence of Cr on the charge distribution in the vicinity of the vacancy we compare the plots of the electron density maps for FeAl phase with the vacancy without Cr and the same when Cr occupies the closest to the vacancy Fe site. As may be seen from Fig. 6, when Cr substitutes for Fe near the vacancy this atom attracts more his own electrons and the density of the charge localized between Cr and the vacancy increases as compared with the non-alloyed case. This result corresponds the behaviour of Cr on-site DOS discussed above.



a b

Figure 6. Electron density map in (100) plane with the vacancy on the Fe site for (a) *FeAl (B2)* phase (b) *FeAl (B2)* phase with *Cr* substituting fot *Fe*

4. Summary

Summing up, we show in this paper that Cr atoms alloying FeAl (B2) phase have amphoteric properties and their behaviour in this phase is rather complicate. The site preference for Cr to occupy the sites in this phase strongly depends on the existence of vacancies. We know these vacancies that are formed on the Fe sites in the lattice. The results of our *ab initio* calculations demonstrate that in these conditions Cr prefers to occupy the closest to the vacancy Fe site, although in the absence of the vacancies these atoms have a slight preference to occupy Al positions. We found that the energy of vacancy formation in FeAl phase is higher than the energy of vacancy formation in FeAl phase when Cr substitutes for Fe, but lower than that in FeAl phase when Cr substitutes for Al. The comparative analysis of the electronic properties in this system allows conclude that such behaviour of Cr atoms is dictated by the peculiarities of the band structure and by the electron charge redistribution caused by the vacancy formation. It is defined by the fine details in the interaction of the *d*-electrons of Fe and Cr atoms in the vicinity of the vacancy.

Acknowledgments

The German-Israeli Foundation supported this work for Scientific Research and Development, grant N^0 G 617-16.10/1999. Authors are thankful to Prof. H.Mehrer for providing the experimental data and constant interest in their work and to Prof. A.Kiv for useful discussions.

References

[1] Stoloff N.S., Sikka V.K. (1996) *Physical Metallurgy and Processing of Intermetallic Compounds*. Chapman and Hall: New York.

[2] Westbrook J.H., Fleischer R.L. (1995) *Intermetallic Compounds: Principles and Practice*. Chichester: Wiley.

[3] Wasilewski R.J. (1968) Structure Defects in CsCl Intermetallics Compounds–I Theory, *Journal of Physics and Chemistry of Solids,* **29**, pp.39-49.

[4] Fu C.L., Zou J. (1995) Site Preference of Ternary Alloying Additions in FeAl and NiAl by First-Principles Calculations, *Acta Metallurgica*, **44**, No.4, pp.1471-1478.

[5] Jansen R. W., Klein B. M. (1989) Pseudo-Atom Calculation of Energies in Metal, *Journal of Physics: Condensed Matter*, **1**, No.44, pp.8359-8368.

[6] Hohenberg P., Kohn W. (1964) Inhomogeneous Electron Gas, *Physical Review*, **136**, No.3B, pp. B864-B871.

[7] Kohn W., Sham L.J. (1965) Self-Consistent Equations Including Exchange and Correlation Effects, *Physical Review*, **140**, No.4A, pp. A1133-A1138.

[8] Blaha P., Schwarz K., Madsen G., Kvasnicka D., Luitz J. (2002) Computer Code WIEN2k, Inst. f. Materials Chemistry, TU Vienna.

[9] Perdew J.P., Burke K., Ernzernhof M. (1996) Generalized Gradient Approximation Made Simple, *Physical Review Letters*, **77**, No.18, pp.3865-3868.

[10] Lechermann F., Welsch F., Elsässer C., Ederer C., Fähnle M., Sanchez J.M., Meyer B. (2002) Density-Functional Study of Fe_3Al: LSDA *versus* GGA, *Physical Review*, *B* **65**, pp.132101-132104.

[11] Mohn P., Persson C., Blaha P., Schwarz K., Novak P., Eschrig H. (2001) Correlation Induced Paramagnetic Ground State in FeAl, *Physical Review Letters*, **87**, No.19, pp.196401-196404.

[12] Bogner J., Steiner W., Reissner M., Mohn P., Blaha P., Schwarz K., Krachler R., Isper H., Sepiol B. (1998) Magnetic Order and Defect Structure of Fe_xAl_{1-x} Alloys Around x=0.5: An experimental and theoretical study, *Physical Review*, *B* **58**, No.22, pp.14922-14933.

[13] Sundararajan V., Sahu B. R., Kanhere D. G., Panat P. V., Das G. P. (1995) Cohesive, Electronic and Magnetic Properties of the Transition Metal Aluminides FeAl, CoAl and NiAl, *Journal of Physics: Condensed Matter*, **7**, pp.6019-6034.

[14] Dridi Z., Bouhafs B., Ruterana P., Aourag H. (2002) First-Principles Calculations of Vacancy Effects on Structural and Electronic Properties of TiC_X and TiN_X , *Journal of Physics: Condensed Matter*, **14**, pp.10237-10249.

[15] Blöchl P.E., Jepsen O., Andersen O.K. (1994) Improved Tetrahedron Method for Brillouin-Zone Integrations, *Physical Review*, *B* **49**, No.23, pp.16223-16233.

[16] Smithels C. J. (1962) *Metals Reference Book.* London: Butterworth, Vol. II, p.581.

[17] Gonzales-Ormeño P.G., Petrilli H.M., Schön C.G. (2002) *Ab-initio* Calculation of the Formation Energies of BCC-Based Superlattices in the Fe-Al System, *Calphad*, **26**, No.4, pp.573-582.

[18] Fu C.L., Ye Y.-Y., Yoo M.H., Ho K.M. (1993) Equilibrium Point Defects in Intermetallics with the B2 Structure: NiAl and FeAl, *Physical Review, B* **48**, No.9, pp.6712-6715.

[19] Smithels C.J. (1962) *Metals Reference Book.* London: Butterworth, Vol. I, p.199.

[20] Korzhavyi P.A., Ruban A.V., Lozovoi A.Y., Vekilov Yu.Kh., Abrikosov I.A., Johansson B. (2000) Constitutional and Thermal Point Defects in B2 NiAl, *Physical Review*, *B* **61**, No.9, pp.6003-6018.

[21] Kass M., Brooks Ch.R., Falcon D., Basak D. (2002) The Formation of Defects in Fe-Al Alloys: electrical resestivity and specific measurements, *Intermetallics*, **10**, pp.951-966.

[22] Peteline S., Tanguep Njiokep E.M., Divinskiand S., Mehrer H. (2003) Diffusion of Solute Elements in Fe_3Al, *Defect and Diffusion Forum*, **216;217**, pp.175-180.

[23] Mattson T.R., Mattson A.E., Sandberg N., Grimvall G. (2000), Vacancies in Metals: from first-principles calculations to experimental data, *Physical Review Letters*, **85**, No.18, pp.3862-3865.

Received on the 21st of May 2005

Computer Modelling and New Technologies, 2005, Vol.9, No.1, 15-31
Transport and Telecommunication Institute, Lomonosov 1, LV-1019, Riga, Latvia

PHASE-SHIFT FUNCTIONS METHOD FOR NANOCLUSTERS ELECTRONIC STRUCTURE CALCULATIONS IN SOLIDS

YU.N. SHUNIN, A.V. GOPEYENKO

Information Systems Management Institute,
Department of Natural Sciences and Computer Technologies,
Lomonosov 1A, LV-1019, Riga, Latvia
shunin@isma.lv, shunin@mits.lv, via.@latnet.lv
phone: +371 7100593

Presently in semiconductor technologies at the micrometer length scale is being used. However, these technologies have achieved the physical limits. Now the downscaling of semiconductor devices to a new technology at the nanometer length scale is expected. Successful production of nanometer scale devices requires a clear understanding of physical and electronic properties of nanometer scale systems.

Nanoclusters have a wide range of applications that depend on their properties. Different kinds of materials are used in different areas. For example metals that have magnetic properties (such as Fe, Cu) can be used for development of new high-density storage devices. Si and Ge are used in semiconductor technologies to produce different nanometer scale electronic devices.

There is a considerable interest in the geometrical, electronic, and chemical properties of nanoscale clusters. Such clusters represent an intermediate phase of matter, whose material properties are often quite different from either the single-atom or bulk properties of the elements involved. With the current scientific focus on nanotechnology, the field of cluster research has received renewed impetus, as clusters may well provide suitable building blocks for the construction of desirable nanostructures. It is in this context that the quantum transport properties of nanoscale clusters may well prove to be important. The recent advent of molecular electronic systems has opened up a frontier in which atoms, clusters, and/or molecules assume the role of electronic device elements. A progress in this field has been rapid, and already prototypical molecular logic circuits have been constructed in laboratories. However, there are many outstanding problems, which need to be understood. In particular, solid-state calculations for nanoobjects are actually. The main attention in this work is paid to the electronic scattering calculation for atomic clusters, which are the nanobjects.

Keywords: *nanotechnology, nanocluster, Shrödinger equation, phase function, phase shift, potential, tight binding approximation (TBA), nearly free electron approximation (NFEA)*

1. Nanomaterials in Nanoelectronics

1.1. NANOCLUSTERS

Nanotechnologies are developed very fast now. They offer new possibilities in different sciences such as physics, biology, chemistry and other. Different materials are used to form nanoclusters.

Metal nanoclusters containing fewer than ~400 atoms show quantum size effects which give them unique properties and make them interesting candidates for the building blocks of nanostructured materials and nanoelectronic digital circuits. Before such practical applications can be developed, however, the cluster's chemical, thermodynamic, electronic, and optical properties must be delineated. This in turn requires a complete and unambiguous characterization of the cluster's geometrical structure. Recent experiments have been able to grow, and separate in mass, gold clusters down to sizes as small as ~1 nm in diameter (~38 atoms).

This recent improvement in experimental isolation capability to smaller sizes has allowed direct comparison of experimental geometries with theoretical predictions based on unbiased and exhaustive searches for the low-energy minima of clusters using model potentials and refined with first principles calculations.

1.1.1. Au nanoclusters

One of the factors, contributing to this controversy, is the complexity of the potential energy surfaces of Au clusters. The short range of the Au potential leads to a very large number of local minima, making localization of the true global minimum extremely difficult. Since the number of local minima in the

potential energy surface increases rapidly, probably exponentially, with size, this uncertainty becomes even worse for larger clusters. Also, different potential models of the metal bond yield different energy orderings for the lowest-energy isomers.

The disordered states of Au clusters of size 19, 38, 55, and 75 atoms have the largest attraction basins, and, combining this with the fact that they are the most stable of all the configurations at finite temperature, it is predicted that they would be the most probable result of cluster condensation from the gas or liquid. Supporting this prediction, the results of density functional calculations and the fact that, at least qualitatively, the experimental structure factors for Au_{38} and Au_{75} appear most like those generated from the disordered states found in [13] than those from the ordered states. This is in contrast to the conclusions in the existing literature on gold nanoclusters. It is suggested, that previous conclusions, drawn from comparing the experimental data with theoretical predictions were biased because of lack of a complete set of low-energy disordered configurations. The disordered states were not previously isolated because prior searches fixated on finding the global minimum and subtle differences in the form of the potential led to slightly higher energies for the disordered structures. It is suggested that the ordered/disordered controversy concerning the structure of metal nanoclusters resulted from the different repulsive core–attractive range relations of the various potentials used. Further attention should thus be paid to improving the potential model representations of the metal bond and the delineation of subtle differences in these on the predictions of the geometries of the low-energy minima of metal nanoclusters. Finally, it should be mentioned that many other Au clusters between 19 and 75 atoms are also expected to be disordered. Work on verifying this, and determining the effect of the passivation layer on the cluster structures of the experimental samples, although assumed to be small, is now under investigation [13].

1.1.2. Nanoclusters of transition and noble metals

Noble metals are widely used in nanoscience. Clusters of transition and noble metals are interesting for their physical and chemical properties, and for technological applications. In this context, platinum clusters are of great importance because of their role in many catalytic processes. The starting point for understanding cluster properties is the determination of their structure, which is usually a nontrivial task, since clusters can assume a wide variety of structures. The simplest ones are pieces of the bulk crystal lattice, which is fcc for noble metals and Pt. Clusters can present also noncrystalline structures, such as icosahedra (Ih) and decahedra (Dh), having fivefold symmetries. Interatomic distances in Ih and Dh differ with respect to the ideal bulk value, thus giving a volume contribution to the energy that is absent in *fcc* clusters. This volume contribution may be compensated by a lower surface energy: especially Ih structures, which present a close-packed surface and a low surface/volume ratio, can be more favourable than *fcc* structures at small sizes, where surface contributions to the energy are dominant. All these structures can be of special energetic stability at the so-called structural magic numbers, which are the numbers of atoms N needed to complete a perfect cluster of a given symmetry. For example, at N = 13 and 55 perfect Ih, truncated Dh, and *fcc* cuboctahedra (Oh) are obtained. Several different calculations indicate that nickel, copper, and silver clusters adopt preferentially the Ih structure at N = 55. On the contrary, calculations on gold clusters show a preference for low-symmetry structures. The latter are often called amorphous because their radial distribution functions resemble those of liquid clusters. These findings have been rationalized in terms of the bond order–bond length correlation in metallic systems. In Au, bonds have a much stronger tendency to contract with decreasing coordination than in Ag, Cu, or Ni, and this favors the disordering of the cluster surface. From this point of view, Pt is intermediate between Au and Ag, and its behavior with respect to amorphization is still an open problem.

The amorphization mechanism of icosahedral Pt nanoclusters is investigated by a combination of molecular dynamics simulations and density functional calculations. A general mechanism for amorphization, involving rosette-like structural transformations at fivefold vertices, is proposed. In the rosette, a fivefold vertex is transformed into a hexagonal ring. For icosahedral Pt nanoclusters, this transformation is associated with an energy gain, and their most favorable structures have a low symmetry even at icosahedral magic numbers, and that the same mechanism underlies the formation of amorphous structures in gold.

The calculations show that icosahedral Pt clusters have, indeed, a tendency towards amorphization. The amorphization mechanism, which is effective also in gold clusters and generally in metallic systems with sticky potential and strong bond order–bond length correlation, takes place through the generation of eventually multiple) rosette motifs at the fivefold vertices. The rosette motif allows an efficient relaxation of the internal atoms, which overcomes a surface energy penalty. In the case of platinum, the bond directionality effects due to *d-d* interactions enhanced the driving force, favouring the rosette [6].

1.1.3. Calcium and strontium nanoclusters

Calcium is one of the most abundant elements on earth and is widely used when combined with other elements. Calcium and strontium are soft alkaline-earth metals that display important structural changes under pressure, which are not characteristic of other metals. For small calcium clusters of up to 13 atoms, the structure, energetic, and electronic structure were studied within the all-electron density functional approach. A massive computational effort would be needed to investigate clusters of larger sizes at the same level of calculation. It is therefore important to develop a simplified quantum-mechanical model such as the tight-binding approach that would be well parameterised for clusters containing several tens to hundreds of atoms that reach the nanometre-size regime.

Classical studies to model calcium cluster structures in this size range were carried out based on a parameterisation on bulk calcium properties of the Murrell-Mottram two- and three-body potential. For small clusters with fewer than 20 atoms, this potential overestimates the binding energies and does not predict the quantum mechanically optimised structures for several cluster sizes. For larger cluster sizes containing several hundreds of atoms, a growth following a pattern that fills atomic icosahedra shells was predicted based on the relative abundance observed in the mass spectrum of hot calcium clusters. However, the structural, electronic, and thermodynamic properties of calcium clusters containing tens of atoms are not well characterized. More specifically, it would be interesting if the structure of nanoclusters could be identified experimentally in this size range. Calcium is very reactive, and nanocluster surface characterization is important.

The mass spectra of calcium and strontium nanoclusters display similar features, though not identical. In both spectra, clusters with 34 and 61 atoms are very abundant and can be identified as magic numbers. The strontium mass spectrum shows another magic number at Sr_{82} not observed in the calcium mass spectrum. Indeed, the calcium spectrum shows a not too strong abundance peak at Ca_{80}–Ca_{81}. Additionally, the calcium mass spectrum shows large abundance at Ca_{37}. Other not so pronounced abundant clusters sizes are observed at Ca_{43} and Ca_{52}. However, in contemporary experiments of the same group, the latter were not clearly detected. The lack of more recent experimental data under better-controlled experimental conditions is unfortunate. Our recent studies of strontium clusters, based on the second-moment-approximation (SMA) many-body potential, have predicted that at low but finite temperatures, the symmetric structures Sr_{34} D_{5h} and Sr_{61} Td are magic numbers. Predictions for calcium nanoclusters put forward in this study will be of interest to several experimental groups.

Contrary to the successful parameterisation of the SMA many-body potential for strontium clusters; it was not possible to effectively carry over an equivalent process in the case of calcium. The SMA many-body potential is a classical representation of the tight-binding approach, and recently cluster-based parameterisations of SMA many-body potentials for sodium, potassium, caesium, and rubidium was also produced. Our SMA many-body potentials have further been used in a variety of studies. For example, Calvo and Spiegelmann used the sodium SMA many-body potential to study phase transitions in sodium clusters containing several tens of atoms.

The calcium cluster electronic structure is different from strontium retaining peculiar quantum characteristics at much larger sizes. Following a fitting strategy similar to Sr, and generalizing the tight-binding (TB) parameterisation of bulk calcium, the objectives of this work are (i) to describe a parameterisation strategy of the tight-binding model that contains information on the structure and energy of small clusters, as well as on the energy and band structure of fcc and bcc bulk calcium, and (ii) use the so-fitted TB model to describe the structural and dynamical properties of calcium nanoclusters. This size regime has not been explored for calcium clusters with a simplified quantum-mechanical description. Indeed, considerable work has been done in the past ten years on the issue of the transferability of TB models. TB models constructed from bulk properties were used to study surfaces, or models from selected lattice symmetries were used to study lattices of different symmetries. The applicability of sets of TB bulk-determined parameters to the study of atomic clusters has also been explored. More recently, Xie and Blackman provided a TB model for rhodium within an orthogonal s-p-d basis set, which is transferable from clusters to bulk solid. Calcium is very different from rhodium because of the relatively long-range interatomic forces in the alkaline earths and the extended character of the valence band when compared to transition metals. Our recent TB study of bulk calcium reproduced correctly the metal-nonmetal and fcc-bcc pressure-induced transitions, and thus the application of TB to Ca nanoclusters is promising. For sodium, there has been a simplified TB model with parameters fitted on Na_2 and Na_4 but not on bulk properties. This simplified TB model did not include d-orbital, and the authors find discrepancies between structures calculated with the SMA model and with their TB model for sizes containing more than 40 Na clusters [8].

1.1.4. Silicon nanoclusters

Silicon is another material that is used in nanotechnologies despite it has some drawbacks. It is an indirect band-gap semiconductor. Thus, silicon (Si) has a major drawback: its inability to emit light efficiently, and, furthermore, its weak emission is in the near IR. There is presently a large research effort aimed at exploring physical and chemical means to break silicon's lattice symmetry and mix different momentum (k) states in order to induce a useful level of luminescence and optical gain. The approaches include (1) impurity-induced luminescence (e.g., S, B, Be, Er), (2) alloy-induced luminescence (e.g., Si-Ge-C), (3) porous silicon, and (4) quantum wires and dots (or nanosize clusters). The first two of these approaches are plagued by, among other things, relatively low luminescence intensity at low temperature which becomes vanishing weak at room temperature, whereas the last two, which may be mechanistically related via quantum confinement, have considerable potential but have remained largely uncontrolled and poorly understood. Success in this endeavour is obviously a major challenge to materials science, one that could have profound technological implications.

Because a visible photoluminescence (PL) has been observed from Si nanoclusters, these clusters and their potential are a subject of current interest. Si nanoclusters have been produced by aerosol techniques, plasma deposition, sputtering, spark ablations and grown as colloids, or in glass matrices by a variety of approaches including ion implantation followed by high temperature annealing; however, all of these techniques produce a large distribution of cluster sizes resulting in very broad optical absorption and PL features which limit usefulness and make definitive interpretation in terms of quantum confinement and other mechanisms difficult. To understand the origin of visible PL and other electronic properties of Si nanoclusters, it is necessary to study size-selected nanoclusters and to assess the role of surface recombination. Definitive experimental results will be the key to future scientific progress and practical utilization of this material. From a physics perspective, such studies should lead to a better understanding of quantum confinement of electrons and holes in indirect band-gap semiconductors. Quantum confinement in direct gap semiconductors such as GaAs and CdSe is fairly well understood, but much less is known about confinement in indirect gap materials. The bulk excitonic radius for Si is ~4 nm which suggests that quantum confinement effects should be observed for nanocrystals smaller than this size. A synthesis method based on using inverse micelles as reaction vessels to produce useful quantities of size-selected clusters was developed and this method was used to synthesize a variety of metal and compound semiconductor clusters. These clusters have been remarkable in their size monodispersity and the sharpness and richness of their spectral features, which have demonstrated strong quantum confinement effects [18].

1.1.5. Germanium nanoclusters

Ge is structurally similar to Si. The optical properties of bulk Si and Ge are rather mediocre because the light-emission in the bulk Si and Ge is a phonon-assisted indirect process. Therefore, to improve on the light-emission feature in Si-based materials is a challenge for both technological and fundamental research. A luminescence is a result of a significant overlap in electron and hole wave functions since the strength of the luminescence (i.e., the emission rate and quantum efficiency) depends on the extent of this overlap and the transition probability. A possible means for increasing this overlap for the Si-based materials may be accomplished through, for example, alloying to change the band structure, introducing impurities to produce the intermediate state through which the electron can recombine with the hole, or zone folding to yield the desired *quasi*-direct transition. However, the most important breakthrough in this topic is the observation of visible photoluminescence (PL) from porous Si and Si quantum dots, which opens possibilities for fabricating visible light-emitting devices from Si-based materials. The structural analysis of porous Si is quite difficult. But several measurements have confirmed that the principal feature of porous Si consists of extremely fine structures, which are small enough to exhibit quantum confinement effects. Various theoretical works have been conducted on Si nanowires and Si clusters. They clarified that the quantum confinement effects give rise to a change in the electronic structure and the optical properties and they are the principle mechanism of the blue shift PL in porous Si and Si quantum dots.

Experimental reports indicated that Ge quantum dots embedded in SiO_2 glassy matrices or in porous Si show a strong room-temperature luminescence. Theoretical studies on the structure and stability of Ge clusters, the polarization of small Ge clusters, and the quantum confinement effect on excitons in Ge quantum dots have also been reported. Since Ge has smaller electron and hole effective masses and a larger dielectric constant than the corresponding quantities for Si, the effective Bohr radius of the exciton

in Ge is larger than that in Si, and the quantum confinement effect appears more pronounced in Ge than in Si. These results suggest that Si_nGe_m nanoclusters could be possible candidates for components of nanoscale functional optical devices. In order to understand the physics of Si_nGe_m clusters, an *ab initio* molecular dynamics simulation for Si_nGe_m clusters of an intermediate size was performed, and their electronic and optical properties were systematically studied. There is no doubt that the mismatch effect dominating the electronic and optical properties in $Si_{1-x}Ge_x$ alloys may introduce interesting optical features in Si_nGe_m clusters. But one has to keep in mind that the surface distortion associated with stabilizing the Si_nGe_m clusters will also play an important role. Therefore the competition between the lattice mismatch and the surface distortion is the basic issue in our investigation. For this purpose, Si_nGe_m clusters of an intermediate size with and without the hydrogen passivation were studied. By comparing the results between the two sets of Si_nGe_m clusters, the fact the surface distortion plays an important role in the intermediate size of Si_nGe_m clusters but the mismatch effect dominates when Si_nGe_m clusters of the intermediate size are passivated by hydrogen atoms to eliminate the dangling bonds so as to lessen the effect of the surface distortion was found. The other fact that the latter shows an enhancement of radiative transition and a blue shift in PL was also ascertained.

It should be noted that the simulations of the Si_nGe_m clusters without hydrogen passivation lead to only one of the more stable configurations among a large number of structural isomers. Hence its resulting structural and electronic properties may not exactly represent the corresponding properties of the true ground-state configuration of the Si_nGe_m clusters. However this caveat does not affect the main conclusions of the study, including the role played by the lattice mismatch and the surface relaxation in Si_nGe_m clusters with and without hydrogen passivation, and the enhanced radiative transition in Si_nGe_m clusters [14].

However, the attempts to overcome the drawbacks of Si are being made. The use of Si in optical applications is limited by its small and indirect band gap. However, recent observations of visible photoluminescence (PL) in porous Si and Si ultra fine particles suggest that Si nanoclusters may become a promising material for optical applications, if their electronic and optical properties were well understood. As of now, the mechanism of the observed visible PL is still under debate. Some researchers attribute the PL to quantum confinement effects in the Si nanostructures, while others attribute it to amorphous Si, siloxene, hydrides/polysilanes, and oxygen-related defect centres. Consensus is difficult to reach, especially in the case of porous Si because of the coexistence of a large variety of surface chemistries and structures in this system. In order to shed more light on this matter, it seems useful to first examine more controllable systems, such as silicon nanocrystals (nc-Si), with well controlled surface chemistry and sizes, and silicon oxide nanostructures (an-SiO_x), whose luminescence properties have some similarities to porous silicon. In this paper, it is shown how nc-Si will small size distribution and an-$Si\text{-}O_x$ can be synthesized in a well-controlled environment. The effects of surface aestivation of necks of different sizes with hydrogen or oxygen at different temperatures on the observed PL are presented. Photoluminescence excitation (PLE) spectra and PL decay times of necks and an-Sio_{ux} are reported. A comparison of the many different and common PL properties among the passivity necks and an-Sio_{ux} is included.

The necks, the size of which can be controlled was synthesized. When passivity by hydrogen or oxygen, these necks showed strong infrared and/or visible PL. A model involving absorption in the quantum confined Si cores can best explain the PL properties of these necks and emission due to transition between defect states in the passivation layer. However, a simple band-to-band recombination mechanism within the Si cores cannot be completely ruled out [20].

1.2. PROPERTIES OF NANOCLUSTERS

There are several ways to examine nanoclusters. In the fast evolving field of nanoscience, where size is crucial for the properties of the objects, simple and sensitive methods for the detection and characterization of single nanoclusters and nanocrystals (nano-objects) are needed. The most commonly used optical techniques are based on luminescence. Single fluorescent molecules have been studied and are now routinely applied in various research domains ranging from quantum optics to life science. Yet, fluorescent molecules allow only for short observation times due to inherent photo bleaching. The development of brighter and more stable luminescent objects, such as semiconductor nanocrystals, has remedied some of this shortcoming, but this improvement has come at the price of a strong blinking behaviour.

An interesting alternative to fluorescence methods relies solely on the absorptive properties of the object. At liquid helium temperatures single molecules were initially detected by an absorption technique

owing to the high quality factor of the zero-phonon line which gives a considerable absorption cross section at resonance (few 10^{-11} cm^2). Single ions or atoms isolated in the traps or high Q cavities have been detected by absorption of a probe beam. In general, particles with large absorption cross-sections and short time intervals between successive absorption events are likely candidates for detection with absorption methods.

Metal nanoparticles fulfil both of these requirements: excited near their plasmatic resonance a nanometer sized gold nanoparticle has a relatively large absorption cross section (~$8 \cdot 10^{-14}$ cm^2 for a 5 nm diameter particle) and a fast electron-phonon relaxation time (in the picoseconds range). Since luminescence from these particles is extremely weak, almost all the absorbed energy is converted into heat. The temperature rise induced by the heating leads to a variation of the local index of refraction. Previously, a polarization interference contrast technique has been developed to detect this photo thermal effect. In that case, the signal is caused by the phase shift induced between the two spatially separated beams of an interferometer, where only one of the beams propagates through the heated region, and images of 5 nm diameter gold nanoparticles have been recorded with a signal-to-noise (SNR) ratio ~10. Also, the sensitivity of this technique, although high, is ultimately limited by the quality of the overlap of the two arms of the interferometer as well as by their relative phase fluctuations.

Recently the new, more sensitive, and much simpler method for detecting no fluorescent nanoobjects were introduced. It uses a single probe beam, which produces a frequency-shifted scattered field as it interacts with time modulated variations of the refraction index around an absorbing nano-object. The scattered field is detected by its beat note with the probe field, which plays the role of a local oscillator as in the heterodyne technique. Because this new method is not subject to the limitations mentioned above, a 2 order of magnitude improvement of the sensitivity is achieved compared to the previous photo thermal method. This allows for the unprecedented detection of small absorptive objects such as individual metallic clusters composed of 67 atoms.

The advantages of photo thermal heterodyne detection for absorbing nanoobjects are demonstrated [2]. As any far-field optical technique, it has a wavelength-limited resolution. An interesting challenge would now be to combine the unprecedented sensitivity of the method presented here with the sub wavelength resolution of near-field optical techniques. The study of the physical properties of very small metallic aggregates or non-luminescent semiconductor nanocrystals is now possible at the individual object level. This photo thermal method does not suffer from the drawbacks of blinking and photo bleaching and is immune to the effects of fluorescing and scattering backgrounds. It could be applied to many diffusion and co localization problems in physical chemistry and material science and to track labelled bio molecules in cells [2].

1.3. METHODS OF NANOCLUSTER FORMATION

Several details about the nanocluster formation would be mentioned below. The development of nanoelectronic devices requires controlled fabrication of nanostructures on surface. Two parallel routes have been taken toward this goal: one is the top-down approach, such as nanopatterning, and the other is the bottom-up approach, such as self-assembly. Here, a novel effect of Coulomb charging on coarsening of metal nanoclusters on semiconductor surfaces, which provides a potentially useful method for controlled fabrication of metal nanostructures is demonstrate. The Coulomb effect is ubiquitous in physics, chemistry, and biology. One well-known manifestation of the Coulomb effect on stability of a cluster is Coulomb explosion. It is defined classically by the Rayleigh instability limit, above which an excessively charged cluster becomes unstable and explodes into smaller fragments. For a nanocluster, the critical size for Coulomb explosion depends on the nature of chemical bonding. In this Letter, a novel manifestation of the Coulomb effect on the stability of clusters, the “Coulomb sink” is demonstrated. When a metal cluster is charged on a surface it may not explode, but instead grow its size by “sinking” atoms from its neighbouring clusters to reduce its Coulomb energy. Both theory and experiment, on the phenomena of Coulomb sink with metal nanomesas grown on semiconductor surfaces are elaborated. Charging reduces the chemical potential of a charged mesa relative to its neighbouring neutral mesas. Consequently, it grows at the expense of its neighbours via a coarsening process. Because one can selectively charge any chosen mesa with a controllable amount of charge, Coulomb sink provides a unique and effective method for manipulating growth of metal mesas with a size control up to millions of atoms.

Coulomb sink, leading to cluster agglomeration, is effectively a reversed process of Coulomb explosion, leading to cluster fragmentation. It provides a unique and effective method for manipulating

growth of metal nanoclusters on semiconductor or insulator surfaces with a size control up to millions of atoms [4].

There are the methods that can influence the growth of nanoclusters, for example one of them can define the region where nanoclusters grow. In recent years, an ion implantation has been used to introduce foreign ions into pure or thermally grown silica to form nanoclusters. An attractive feature of ion implantation to form these nanoclusters is that the clusters grow in a well-defined region in the sample, determined by the implantation depth. Most of the scientific effort is focused on the interesting linear and non-linear optical properties of these layers, which can have applications in optical semi conducting devices such as lasers based on Si-technology. The combination of ion implantation and thermally grown SiO_2 is in this respect quite promising since both techniques are employed on a massive scale in semiconductor industry. The physical properties of these nanocrystals differ largely from the normal bulk ones. This can be attributed to both the discreteness of the electronic states for very small clusters as well as to the large influence of the surface of the particle due to its large surface to volume ratio.

Also the vibrational dynamics of the particle change drastically in going to very small cluster sizes. This change will reflect in some of the physical properties of the precipitates such as the thermal heat capacity, the super conducting transition temperature, the melting temperature, and the Mössbauer f fraction. Processes governed by electron-phonon interactions (such as superconductivity) are also influenced by the change in the vibration spectrum.

Numerous attempts have been made to give a good theoretical description for the vibrations of free and embedded nanoclusters, mostly in connection with the effect of the particle size on the specific heat and the Debye-Waller factor. These descriptions are based on a wide variety of models such as the Einstein model, the dynamical matrix model, molecular dynamics, and the elastic-body model. The last model has been especially successful in describing the low-lying vibrational modes for embedded nanoclusters as was shown by low-frequency Raman scattering data. This model is very powerful in describing the complete physical behaviour of a micro crystal embedded in a matrix since it can calculate all vibrational modes with only a few material parameters (the longitudinal and transversal velocity of sound and the density for the cluster and matrix material) [7].

Ion implantation method can also be used to change the nanocluster properties. Ion implantation and subsequent high-temperature annealing is an effective way to prepare metal nanoclusters dispersed in a dielectric for useful optical and electrical properties. However, there is very little understanding of the nucleation and growth process of these nanoclusters, their correlations with the sites of the implanted ions, and the behaviour of defects (such as vacancies) generated during the ion-implantation process.

Materials composed of a high density of metallic precipitates exhibit a large nonlinearity in third-order optical susceptibility at the surface plasma resonance frequency. Thus, the refractive index of a composite can be modified and controlled as a function of light intensity. These materials have potential applications in all-optical-memory and switching devices. Although ion implantation and subsequent high temperature annealing are feasible methods for modifying materials, ion implantation induces a range of defects, such as vacancies, interstitials, and anti-sites. These defects and their clusters critically influence properties of the implanted system. For example, Xu et al. have proposed that transfer of the electrons from the Au cluster surfaces to the quantum antidotes (a subnanometer-scale vacancy cluster) may account for the observed red-shift in gold surface plasma resonance when Au nanoparticles are dispersed in a single crystal MgO. However, little is known about the early stage of the evolution of metal nanoclusters embedded in a dielectric matrix, including such processes as the lattice position of the implanted ion or the nucleation process for forming nanoclusters. This has been because structural features less than ~2 nm and with poor crystalline cannot be analysed by using conventional transmission electron microscopy (TEM) or high-resolution TEM (HRTEM) phase contrast imaging. [9]

Interesting thing is the burrowing of Co nanoclusters on Cu substrate. Recent experiments show that when a system consisting of Co nanoclusters, which land thermally on a Cu substrate, is heated up to 600 K the nanoclusters burrow into the substrate. Transmission electron microscopy measurements performed on such samples showed that the fully burrowed nanoclusters are aligned with the substrate.

This phenomenon could prove to be crucial for the development of new high-density storage devices. Supported magnetic nanoclusters on inert substrates, like noble metals, are considered to be good candidates because they satisfy both the requirements put on novel magnetic materials: size integration and highly localized magnetic moments.

Although the experiments establish the fact that this process exists and energy balance considerations1 indicate that it is energetically favourable for the cluster to burrow, it is not clear what the mechanism of this process is.

The most important question on this matter concerns the burrowing mechanisms, what kind of mechanisms are involved and how they apply on different cluster configurations. The answer to this question could play a significant role in the optimisation of the manufacturing process of nanostructured films of this nature.

How and when the nanocluster aligns up with the substrates lattice is certainly also an interesting question. For an alignment of crystals with different lattice constants to be possible, the lattice constants should not differ more than ~3%. This is certainly the case for Cu and Co where the difference is ~2%. Burrowing of Co nanoclusters on Cu has previously been examined by means of quasi– *ab initio* molecular dynamics (MD) simulations. These works examine very small clusters, consisting of tens of Co atoms, which are burrowed into the Cu substrate. The main conclusions of these works are that the magnetic properties of the nanocluster would play a significant role in the burrowing process and that the cluster completely loses its initial shape. As it is shown in this paper, nanoclusters larger than ~1 nm in radius will show a different behaviour due to the higher structural integrity [11] .

One of the perspective ideas of nanoclusters development is alloying which can extend the variety of nanoclusters properties. One of the questions is could the size of nanocluster being alloyed influence the properties of alloyed cluster.

Isolated metal nanoclusters offering the prospect of being used as building blocks in the rapidly developing field of nanotechnology recently have attracted much interest. Presently, however, size-selected clusters are mostly elemental and restricted in diameter to below 2 nm if prepared with atomic precision. Naturally, one would like to extend this class of materials to include compounds and alloys for free as well as supported clusters. In the latter case, a prominent recent example is FePt nanoparticles, which are candidates with a potential for ultrahigh density data storage applications due to their ferromagnetic behaviour at room temperature as opposed to pure Fe clusters of the same size, which are strongly fluctuating super paramagnets. Of similar importance are semiconductors quanta dots like CdSe nanocrystals offering attractive optical properties or bimetallic core shell particles leading to extraordinary catalytic behaviour different from that of the pure shell metal.

Although alloy clusters are very attractive objects due to the extended variety of their properties, understanding the process of alloying for feature sizes approaching the molecular limit, central for the development of multi component nanoscaled devices, still remains a challenging task. On one hand, alloy formation has been predicted theoretically and found experimentally even for metals known to be immiscible in the bulk phase after reducing their particle size (critical size: 2–3 nm). On the other hand, surface-segregated, core-shell nanoparticles could be produced in systems like Pd-Ag, which are known to be fully miscible in the bulk phase.

In the special case of Au nanoparticles (size >3 nm) rapid alloying was found experimentally and explained theoretically as being due to surface melting even at room temperature in bimetallic systems with a large negative heat of mixing like Cu or Sn after vapour deposition onto Au nanoparticles kept at ambient temperature. In addition, alloying within a surface layer of 3–4 nm has been reported during the deposition of In atoms on top of Au films even at cryogenic temperatures. Assuming a similar reaction depth for Au nanoparticles as for Au films, one expects a complete intermixing and alloy formation for particle sizes below 3 nm.

Such an expectation, however, neglects all changes in the electronic density of states induced by the electron confinement. In the size range studied here (0.8–2.9 nm), quantum size effects lead to a transition from a ‘‘bulk like’’ (metallic) to a ‘‘molecular’’ (insulating) behaviour [18] when starting with larger clusters and progressing towards smaller ones. The diameter range where this transition is expected can be experimentally narrowed down to particle sizes between 1.4 nm (clusters containing 55 atoms) and about 1.2 nm (clusters containing 33 atoms), the former being electronically in a metallic state while the latter were found in an insulating molecular state.

Thus, one concludes that the size dependent electronic properties of the Au nanoparticles are not decisive of whether the alloy formation into $AuIn_2$ does occur: Despite the 0.8 nm Au clusters behaving molecularly prior to the indium deposition rather than metallically as the particles above 1.6 nm do, they all react completely into $AuIn_2$; i.e., the quantum size effects in the electronic structure of the nanoclusters obviously do not play an important role. For applications in nanoscience this is promising news, since it opens the prospect of *a posteriori* manipulation and tailoring of metallic nanoobjects by their subsequent alloying. On the other hand, the present results underline the striking stability of the ‘‘magic-number’’ Au_{55} clusters against alloy formation despite the existence of a large negative heat of mixing in the Au-In system acting as a strong driving force. Considering the above stated independence of the alloy formation

to the detailed electronic properties of the reacting Au nanoparticles, this extraordinary stability must be exclusively related to the structural closing of the packing shell of these nanoobjects. This, in turn, makes Au_{55} clusters attractive as chemically inert building blocks for new nanoscaled devices. Thus, the present results concerning the alloy formation in metallic nanoparticles offer a new design tool for tailoring properties of nanoobjects [1] .

Although alloy clusters have many perspectives for the development, there are also the problems concerning the modelling of such clusters.

Studies of site-specific compositional variations in small alloy clusters are relevant to both basic research and potential catalytic, magnetic, or other applications. For example, the high chemical reactivity and selectivity anticipated for low coordinated sites, such as vertexes and edges, should be affected by their elemental composition. In view of limitations of currently available experimental tools, theoretical modelling of clusters has gained a central position in acquiring atomic-scale compositional and structural information.

Two statistical-mechanical approaches, each with its advantages and drawbacks, were applied in calculations of site specific compositions in binary alloy clusters (multi component alloy clusters have not been hitherto studied to our best knowledge). The first approach applies computer simulations, while innately taking into account many-particle correlations and facilitating use of rather realistic energetic models based on pair or many-body potentials, derived empirically or from electronic structure of alloys. However, computer simulations are time consuming and typically provide results only for quite limited sets of temperatures and compositions of alloy clusters. This may impede systematic studies of site-specific compositions in clusters and even overlook details of segregation and ordering trends. The second approach, used in a few early works, is based on the analytical Bragg-Williams (BW) approximation that entirely neglects interatomic correlations (short-range order) [12].

Another aspect in nanoscience that under development concerns ordered arrays of nanoclusters.

They are promising materials for next generation microelectronics, ultra-high-density recording and nanocatalysis. A self-organization in heterogeneous strained thin-film growth and self-assembly in chemical synthesis are two of the most commonly used methods to obtain such nanostructures spontaneously. No method has succeeded in producing reproducibly identical nanoclusters/dots with periodic spatial distribution, which is highly desirable for practical device applications and is an open question in molecular and solid-state physics of these “artificial atoms”. A fabrication of uniform-size cluster arrays at the ultrasmall 1–2 nm size regime is even more challenging because fluctuation at a level of only a few atoms could substantially alter their electronic properties. On the other hand, ultrasmall cluster arrays of such dimension have potential for quantum application because the Fermi wavelength for most metals is around 1 nm. At such a length scale, one could also maximize quantum confinement effects and test the fundamental limitations that such effects could impose on the electronic properties. Self-assembly of nanoclusters on periodic solid surface has been shown to be a promising approach to the problem, however, growth of ordered arrays of nanoclusters with identical size and tuneable composition is still a daunting challenge.

Certain clusters with a specific (magic) number of atoms exhibit electronic and/or atomic closed-shell structures and hence remarkable stability. For substrate-supported clusters, while the “closed-shell structure” is still under debate, several recent studies suggested that supported clusters of specific or “magic” sizes indeed exist with remarkable stability against others. As the substrate could interact with the clusters, a substrate modification of the magic sizes may be unavoidable. On the other hand, such an interaction could play a pivotal role by automatically selecting identically sized clusters that for gas phase has to be done by mass spectrometry.

The method for fabricating “customized” highly uniform nanocluster arrays on Si(111) with atomic precision is quite efficient. The physical origin of the stable or magic sizes that makes the method possible is established and the atomic structures for the In clusters are determined by first-principles calculations. The ability to assemble nanoclusters and the thermal stability up to 200 ±C for the nanocluster arrays on Si allow for integration with existing microelectronic architectures. Finally, the ability to form magnetic and/or alloyed nanocluster arrays may lead to breakthroughs in other important areas such as surface nanocatalysis and nanomagnetism [17].

Nanosystems in solids are a very perspective structures for modern electronics. But the large amount of configuration demands considerable theoretical efforts to find optimal atomic configurations in nanoclusters. Electronic properties of such systems play the main role for modern nanoelectronic devices.

2. Electronic Structure Calculations in Solids in the Multiple Scattering Approach

Every electron in a crystal moves within in a complicated potential field, which is created by atoms and by moving electrons. The Schrödinger equation is the basement for start analysis. To solve Schrödinger equation for electron in the crystal and, thus, to find the system of electronic states for the electron is very difficult and at the present time some various approaches and methods are used. But there are only two basic conceptual approximations: *Tight Binding Approximation* (TBA), *Nearly Free Electron Approximation* (NFEA).

In TBA it is taken into account that the energy of interaction of electron with its atom is much larger than the interaction energy with the other atoms. In the other words the electrons are strongly connected to their atom, on which the other atoms exert small influence with their electromagnetic fields only splitting their energetic levels. In such a way atom levels are split under the impact of the outer magnetic field. In this case the atoms interaction with each other only slightly changes the picture of electrons energetic levels of isolated atom.

In the context of NFEA it is considered that the electron moves "almost freely" in the weak potential of ion core, which is considered as light perturbation. In this case the kinetic energy of electron considerably exceeds the interaction of this electron with ions. This approximation is the basement of multiple scattering approaches for electronic structure calculation.

2.1. POTENTIAL CALCULATIONS

To calculate electronic charge density it is necessary to find an effective procedure to calculate a potential. To carry out these calculations several methods could be used. The first one is Matheiss-Wood method where nucleus and electron parts of the potential are parted. The same idea is used in Xα - Slater method. The α parameter is an adjusting parameter and is chosen accordingly to consist the electron total energies received as a result of Hartree-Fock procedure with energies that where calculated using the Xα - Slater method. In this method main factors that define the level of the potential energy of the electron in one-electron approximation should be taken into the consideration. The main calculations should be aimed to calculate a nucleus part of the potential and an electronic charge density distribution near the nucleus, which is used to calculate exchange contribution:

$V_{x\alpha} = -6\alpha\left(\frac{3}{8\pi}\rho\right)^{\frac{1}{3}}$ in Xα-method.

The next step is the MT-approximation of the potential. The MT-approximation allows to divide a complicated superposition of the potentials into the system of isolated potential wells, which are interlinked by the constant level of the interatomic energy (MT-zero).

2.2. ATOMIC POTENTIALS

The potential of neutral atom could be written as the sum of the potentials of nucleus and electron parts:

$$V_{cr}(\mathbf{r}) = V_{coul}(\mathbf{r}) + V_{xs}(\mathbf{r}) . \qquad (1)$$

It is convenient to use the analytical *Gaspar* potential for nuclei, as it is the universal approximation of the electrostatic screened potential (Coulomb part). The main advantage of this potential is that it approximates numerical calculations of the potential within *Thomas-Fermi* method in wide-range of charge numbers **Z** very well and at the same time it is an analytical function:

$$V_{coul}^{G} = -\frac{2Z\exp(-\lambda r/\mu)}{r(1+Ar/\mu)} \quad , \qquad (2)$$

where λ=0,1837, μ=0,8853$Z^{-1/3}$, A= 1,05**.**
Then it is possible to find electronic charge density using Mattheiss-Wood idea:

$$V_e(r) = 2Z/r - V^G(r) , \qquad (3)$$

$$\rho(r) = \nabla_r V_e / 8\pi \,, \tag{4}$$

where $V_e(r)$ is the screened part of the potential, $\rho(r)$ is the electronic charge density.
Then the exchange term in static approximation is:

$$V_{x\alpha} = -6\alpha\left(\frac{3}{8\pi}\rho\right)^{\frac{1}{3}}. \tag{5}$$

The α parameter is an adjusting parameter and is chosen accordingly to consist the electron total energies received as a result of Hatree-Fock procedure with energies that where calculated using the Xα – Slater method. These calculations were made by Schwartz for the Z=1, 2…41, but should be noted that for large Z, α ~ 0.7 and decreases slowly. This method is very simple, but it has one weak point, the α parameter itself. Therefore German and Schwartz (Xαβ-method) made the modification to this method. The advantage of this method is the constant parameters α, β for any Z. α=0,66(6) and β=0,003,
where

$$V_{X\alpha\beta} = [\alpha + \beta G(\rho)]V_{xs} \,,$$

$$V_{xs} = -6\left(\frac{3\rho}{8\pi}\right)^{\frac{1}{3}} \,, \tag{6}$$

and, where the gradient expansion of electronic charge density

$$G(\rho) = \frac{4}{3}\left(\frac{\nabla\rho}{\rho}\right)^2 - 2\frac{\nabla^2}{\rho}\rho \tag{7}$$

is used. Equations (1), (2), (5) give an analytical expression for the potential of the isolated atom and this is very convenient for the numerical equations.

2.3. “CRYSTALLINE” POTENTIAL

The usage of isolated atoms potentials in MT-approximation at electronic structure of solids calculations is incorrect as it is necessary to take into consideration the influence of short range ordering. That is why it necessary to build so called “crystalline” potential. The term “crystalline” means that it is used to describe potential energy of electron in the field of nuclei and other electrons. The basis to formulate the “crystalline” potential is the isolated atom potential. In this case the Mattheiss-Wood idea about the separate interpretation of nucleus and electron parts is used. The superposition of ion cores potentials for single bond can be written as:

$$V_{cr.coul}(r) = V_{coul}(r) + V_{coul}(a-r) \,, \tag{8}$$

where *a* is the interatomic distance.
The exchange part of the potential can be presented in the following way:

$$V_{X\alpha}(r) = -6\alpha\left[3\rho_{cr}(r)/8\pi\right]^{1/3} \,, \tag{9}$$

where electron charge crystalline density using (2-6) is:

$$\rho_{cr}(r) = \rho(r) + \rho(a-r) \,. \tag{10}$$

If it is necessary V_{coul} and ρ_{cr} could be defined more precisely with the help of known Lewdin α-functions, i.e. to take into account the effect of several neighbours, however it should not be mentioned in the first approximation. Then, the needed “crystalline” potential could be found from the following equation:

$$V_{cr}(r) = V_{coul}(r) + V_{xs}(r) \,. \tag{11}$$

So “crystalline” potential is an analytical function, which is easy to calculate.

2.4. POTENTIAL MT-APPROACH

As it was written above, potential MT-approximation allows replacing a complicated combination of intersecting potentials by the system of isolated MT-potentials with spherically symmetric MT-potentials in interatomic medium, which is characterised by the constant potential level (MT-zero). “Crystalline” potential should be cut at the distance equal to the half of the distance to the nearest neighbour $R_{MT} = \frac{1}{2}a$. Then MT-potential could be produced from (11):

$$V_{MT}(r) = V_{cr}(r) - V_{MT0}\,, \tag{12}$$

which should be considered as a spherically symmetric function. V_{MT0} characterizes peculiar energetic border between localized and non-localized states, but this margin is quite conventional. Non-trivial in the usage of MT-approximation is the choice and the proof of MT-zero level. If in metals where there is good screening it is considered that it is reasonable to use averaged level of potential energy in interatomic space then to the semiconductors and dielectrics it is not satisfactory because of strongly changing level of the potential outside the MT-spheres.

2.5. PHASE SHIFTS

An electronic structure calculation is considered here as a scattering problem, where centres of scattering are atoms of clusters. The first step of modelling is the construction of potentials, both atomic and crystalline. To obtain the electronic structure, the calculation of scattering properties is necessary. Scattering properties of these potentials are calculated in form of phase shifts δ_l,

The “crystalline” potential will be used for logarithmic derivatives calculation $\gamma_l = R_l^{'}(r) \big/ R_l(r)\Big|_{R_{MT}}$

by numerical integration of Shrödinger radial equation:

$$\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dR_l}{dr}) + [k^2 - \frac{l(l-1)}{r^2} - U(r)]R_l = 0\,. \tag{13}$$

The numerical integration is made using the forth-order Runge-Kutt method. The peculiarity of this calculation is that the integration interval 0-RMT is divided into two parts: the small values of r, where we have to ensure the singularity of this potential and the solution of this equation is $R_l = r^l\varphi(r)$ and where the equation (3.13) for the $\varphi(r)$ function looks like:

$$\varphi''(r) + \frac{2}{r}(l+1)\varphi'(r) + [k^2 - U(r)]\varphi(r) = 0\,, \tag{14}$$

and the large values of r, the potential weak-change region, where (14) was integrated. After this we will receive the logarithmic derivatives and calculate the phase shifts for the single scatterer in vacuum:

$$tg\delta_l = \frac{kj_l'(kR_{MT}) - \gamma_l j_l(kR_{MT})}{kn_l'(kR_{MT}) - \gamma_l n_l(kR_{MT})}\,. \tag{15}$$

2.6. PHASE FUNCTION METHOD

There are different models of electronic wave scattering in condensed matter. First of all we will define main positions of our scattering model. We assume that plane electronic wave e^{ikr} interacting with a single atom or medium transforms into studied wave that can be expanded in to wave train as follows:

$\Psi_{nlm} = \sum_l R_{nl} Y_l^m$. Phase function methods allow solving the scattering problem directly, integrating the special phase shifts equation:

$$\frac{d}{dr}\delta_l(r) = -\frac{1}{k}V(r)[\cos\delta_l(r)j_l(kr) - \sin\delta_l(kr)n_l(kr)]\,. \qquad (16)$$

Further procedure of electronic structure calculation in effective medium approximation (in this consideration – *Coherent Potential Approximation*, CPA) looks as follows.

Let's locate spherical "potential box" that is in the vacuum in the environment the properties of which are modulated with the "effective" complex energy-dependent potential. Physically, the presence of such an environment should ensure damping of the outgoing wave. The damping of the wave is related to complex wave number and outgoing wave in effective environment in infinity is $h_l^{(+)}(kr) \sim e^{ikr}/kr$. But as $F_l=N_l+A_lJ_l$, where F_l is linear combination of functions:

$$J_l = \cos\delta_l j_l(kr) - \sin\delta_l n_l(kr) \text{ and } N_l = -\cos\delta_l n_l(kr) + \sin\delta_l j_l(kr)$$

and A_l is complex coefficient) also connects outgoing wave it is necessary to search A_l from condition of logarithmic derivative $h_l^{(+)}$ and $F_l=N_l+A_lJ_l$ equality:

$$k\frac{N_l^{'}(kR) + A_l J_l^{'}(kR)}{N_l + A_l J_l} = K\frac{h_l^{(+)'}(KR)}{h_l^{(+)}},$$

where R is the boundary of a spherical "potential box". However, the search of A_l is impossible, while the dispersion law of effective environment *E-K* is unknown. The dispersion law *E(K)* could be received from the following equation:

$$\frac{1}{k}\sum_l (2l+1)\exp(i\delta_l(\mathbf{k},E))\sin\delta_l(\mathbf{k},E) = 0,$$

where $\delta_l(k,E)$ is the complex phase shifts, which characterize the scattering and attenuation in effective medium. After that it is possible using to obtain the expression for the "one-atom" cluster density of electronic states (EDOS) in effective medium as:

$$\rho(E) = \frac{2}{\pi}\sum_l (2l+1)\left[\frac{d\delta_l}{dE} - \frac{R^2 J_l^2(kR)}{2}\frac{\partial\gamma_l(k,\delta_l)}{\partial k}\right]\mathrm{Im}\,A_l\,,$$

where R is the cluster radius, J_l is the combination of Bessel and Neumann functions, γ_l is the logarithmic derivative of wave function on the cluster boundary, which is connected with the δ_l, A_l is a coefficient of self-consistency of cluster volume with the external effective media.

The proposed method of atomic potential approximation gives a satisfactory concordance with self-consistent calculations of *Xα*-Slater method for a wide range of atoms moreover at the same time the economy of machine time is achieved. "Crystalline" potential in MT0-approximation based on the atomic potential calculations could give the real phase shifts. The choice of interatomic energy as the MT-zero in the point of contact of MT-spheres is principal as it explicitly determines the energetic scale shift and the position of all peculiarities of electronic structure. The phase function method possesses a lot of advantages. In particular, it is essential that the equations of this method be formulated directly for observable values, i.e. for phases and amplitudes of scattering. The effective medium approach gives a possibility to take into account various integral scattering cases for solids, namely both as crystalline as amorphous.

3. Phase shifts calculations for nanoclusters

The results of the phase shift calculations on the basement of phase shift equation (16) have been fulfilled for some model nanocluster and realistic potentials (Si, C, Fe). All calculations were made on the basement of programming in **Matlab** mathematical package. The integration of the equation (16) is rather rational. The phase shifts are calculated directly without a traditional integration of Shrödinger equation.

This means smaller numerical integration errors.

3.1. INVESTIGATIONS OF PROPERTIES OF PHASE SHIFT EQUATION

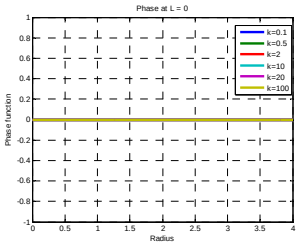


Figure 1. Phase shifts for zero potential field

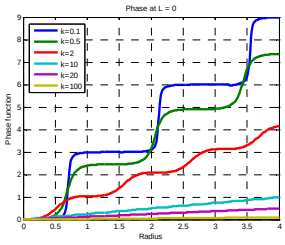


Figure 2. Phase shifts for positive constant field

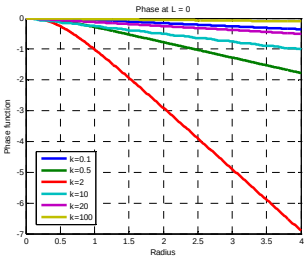


Figure 3. Phase shifts for negative constant field

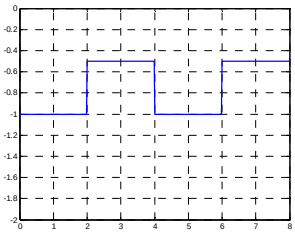


Figure 4. Model nanocluster potential

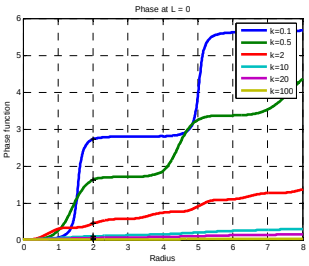


Figure 5. Phase shift functions L=0

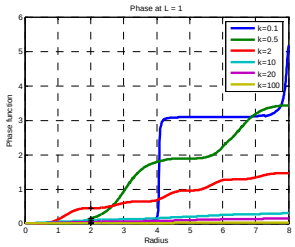


Figure 6. Phase shift functions L=1

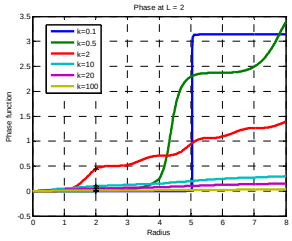


Figure 7. Phase shift functions L=2

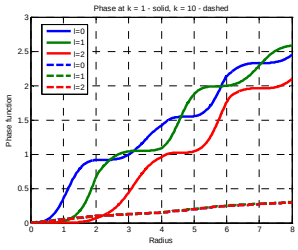


Figure 8. Phase functions L=0,1,2

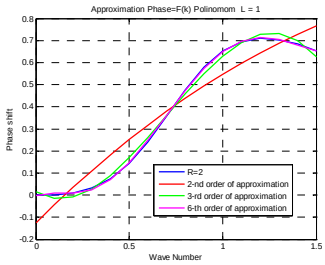


Figure 9. Phase shift functions L=1 via the wave number

The mathematical properties of the equation (16) for evident simple potential fields have been made. The model plain potential values are: 0 Ry , -5 Ry and +5 Ry. As it is seen from the Figure 1 the phase function value for all values of radius is equal to zero. For negative values of the potential the phase functions are positive and for positive potential they are negative.

For more complicated step-type potential (Figure 4) the calculation results looks as it is presented on Figures 5,6,7,8. The Figure 9 demonstrates the typical dependence of the phase shift $\delta_l(k)$,. that is necessary for electronic structure calculations.

3.2. PHASE SHIFTS CALCULATIONS FOR REALISTIC ATOMIC CLUSTERS

The calculations can be divided in some parts. The first part is the calculations of potentials according above-described procedure: Coulomb potential, exchange potential in Xα-approximation for, "crystalline" potential, MT0-potential and also the electronic charge density. Atomic potential was calculated using the equation (1), for "crystalline potential" equation (11) was used and MT0-potential was found using the equation (12). For all these equations the radius argument has been varied from zero to covalent radius of an atom. The typical result of these calculations for Si, as an example, is presented on the Figure 10. Figures 11,12 present calculation of phase shift functions via the radius.

To find the phase shifts functions $\delta_l(k)$, it is necessary to make a cut of the phase function values at a certain radius of integration. This cutting radius means an effective radius of a scatterer. In this case it was at *R=2* (see Figures 13,14,15). But, for more complicated potential field (nanocluster potential) this radius should be estimated especially.

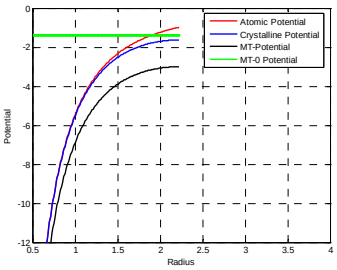


Figure 10
Potential for silicon

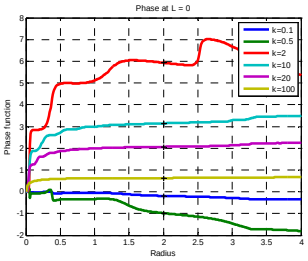


Figure 11
Phase shift functions L=0

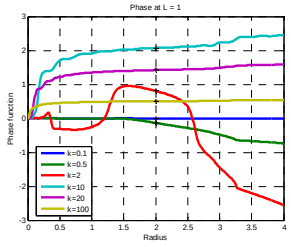


Figure 12
Phase shift functions L=1

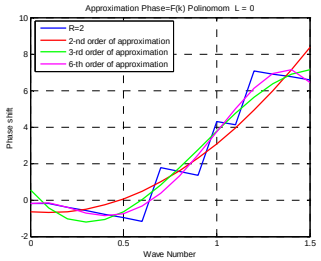


Figure 13. δ(k) function graphic for silicon at radius R=2 for different approximation order at L=0 order

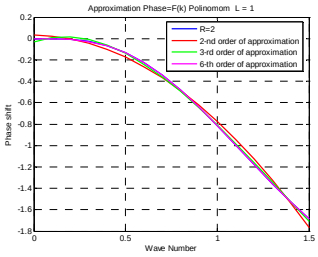


Figure 14. δ(k) function graphic for silicon at radius R=2 for different approximation order at L=1 order

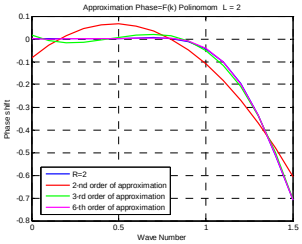


Figure 15. δ(k) function graphic for silicon at radius R=2 for different approximation order at at L=2 order

Conclusions

This work presents the first step of the electronic properties of nanoclusters calculations in solids. The main calculations have been devoted to the modelling of the potentials in the framework of MT-potential approximation. The "crystalline" potential has been used to receive phase functions directly from the phase shift equation. This is an essential advantage of the scattering theory.

Using these results it is possible in principle to continue the study of the electronic properties of atoms and atomic clusters. The next step is the calculations of the electronic density of states, and then the total energy of atoms and atomic clusters. These calculations are necessary for calculation of the scattering properties of the single atoms or nanoclusters.

Applications of scattering theory concepts and technique allow describing the behaviour of electrons in condensed matters in many aspects. These applications can be very fruitful, but the large experience of calculations and analyses are necessary.

The general results can be formulated as follows.

- Nanosystems in solids is a very perspective structures for modern electronics. But the large amount of configurations demands considerable theoretical efforts to find optimal atomic configurations in nanoclusters. Electronic properties of such systems play the main role for modern nanoelectronic devices.
- The proposed method of atomic potential approximation gives a satisfactory concordance with self-consistent calculations of $X\alpha$-Slater method for a wide range of atoms moreover at the same time the economy of machine time is achieved.
- "Crystalline" potential in MT0-approximation based on the atomic potential calculations could give the realistic phase shifts.
- The choice of interatomic energy as the MT-zero in the point of contact of MT-spheres is principal as it explicitly determines the energetic scale shift and the position of all peculiarities of electronic structure.
- The phase function method possesses a lot of advantages; in particular, it is essential that the equations of this method are formulated directly for observable values, i.e. for phases and amplitudes of dispersion.
- The effective medium approach gives a possibility to take into account various integral scattering cases for solids, namely both as crystalline as amorphous.
- Parametric model phase shift calculations demonstrate main tendencies of phase functions behaviour. This simplifies the analysis of more complicated cases of scattering. Realistic potentials phase shifts, which may be calculated in the framework of developed method of

solution of phase shift equation, are the basement for electronic structure calculation of atoms and nanoclusters.

- The procedure of realistic calculation is rather convenient as it uses special realistic analytical potential. This simplifies integration of phase shift equation and gives more precise results.

Acknowledgments

The Grant No.04.1039 of Latvian Council of Science supported this work.

References

[1] Boyen H.-G., Ethirajan A., Kästle G., Weigl F., Ziemann P., Schmid G.. Garnier M. G, Büttner M., Oelhafen P. (2005) Alloy Formation of Supported Gold Nanoparticles at Their Transition from Clusters to Solids: Does Size Matter? *Physical Review Letters*, **94**, 016804.

[2] Berciaud S., Cognet L., Blab G.A., Lounis B. (2004) Photothermal Heterodyne Imaging of Individual Nonfluorescent Nanoclusters, *Physical Review Letters*, **93**, 257402.

[3] Gonzalez J.I., Lee T.-H., Barnes M.D., Antoku Y., Dickson R.M. (2004) Mechanical Single-Gold-Nanocluster Electroluminescent Light Source at Room Temperature, *Physical Review* Letters, **93**, 147402.

[4] Han Y., Zhu J.Y., Liu F., Li S.-C., Jia J.-F., Zhang Y.-F., Xue Q.-K. (2004) Sink: A Novel Coulomb Effect on Coarsening of Metal Nanoclusters on Semiconductor Surfaces, *Physical Review Letters*, **93**, 106102.

[5] Zheng J., Zhang C., Dickson R.M. (2004) Highly Fluorescent Water-Soluble, Size-Tuneable Gold Quantum Dots, *Physical Review Letters*, **93**, 077402.

[6] Aprà E., Baletto F., Ferrando R., Fortunelli A. (2004) Amorphization Mechanism of Icosahedral Metal Nanoclusters, *Physical Review Letters*, **93**, 065502.

[7] Koops G.E.J., Pattyn H., Vantomme A., Nauwelaerts S., Venegas R. (2004) Extreme Lowering of the Debye Temperature of Sn Nanoclusters Embedded in Thermally Grown SiO_2 by Low-lying Vibrational Surface Modes, *Physical Review B*, **70**, 235410.

[8] Dong X., Wang G.M., Blaisten-Barojas E. (2004) Tight-binding Model for Calcium Nanoclusters: structural, electronic, and dynamical properties, *Physical Review B*, **70**, 205409.

[9] Wang C.M., Shutthanandan V., Zhang Y., Thevuthasan S., Duscher G. (2004) Direct Observation of Substitutional Au Atoms in $SrTiO_3$, *Physical Review B*, **70**, 172201.

[10] Cougo dos Santos M., Geshev J., Pereira L.G., Alves M.C.M., Schmidt J.E., Allongue P. (2004) Intralayer Coupling in Self-organized Fe Nanoclusters Grown on Vicinal Si(111), *Physical Review B*, **70**, 104420.

[11] Frantz J., Nordlund K. (2003) Mechanism of Co Nanocluster Burrowing on Cu(100), *Physical Review B*, **67**, 075415.

[12] Rubinovich L., Polak M. (2004) Site-specific Segregation and Compositional Ordering in Ni-based Ternary Alloy Nanoclusters Computed by the Free-energy Concentration Expansion Method, *Physical Review B*, **69**, 155405.

[13] Michaelian K., Rendón N., Garzón I.L. (1999) Structure and Energetic of Ni, Ag, and Au Nanoclusters, *Physical Review B*, **63**, pp.2000-2010.

[14] Yu M., Jayanthi C.S., Drabold D.A., Wu S.Y. (2003) Enhanced Radiative Transition in SinGem Nanoclusters, *Physical Review B*, **68**, 035404.

[15] Yakimov A.I., Dvurechenskii A.V., Nikiforov A.I., Ulyanov V.V., Milekhin A.G., Govorov A.O., Schulze S., Zahn D.R.T. (2003) Stark Effect in Type-II Ge/Si Quantum Dots, *Physical Review B*, **67**, 125318.

[16] Roland Ch., Meunier V., Larade B., Guo H. (2002) Charge Transport through Small Silicon Clusters, *Physical Review B*, **66**, 03533.

[17] Li J.-L., Jia J.-F., Liang X.-J., Liu X., Wang J.-Z., Xue Q.-K., Li Z.-Q., Tse J.S., Zhang Z., Zhang S.B. (2002) Spontaneous Assembly of Perfectly Ordered Identical-Size Nanocluster Arrays, *Physical Review Letters,* **88**, 066101.

[18] Wilcoxon P., Samara G.A., Provencio P.N. (1999) Optical and Electronic Properties of Si Nanoclusters Synthesized in Inverse Micelles, *Physical Review B*, **63**, pp.2704-2714.

[19] Dinh L.N., McLean II W., Schildbach M.A., Balooch M. (1999) Synthesis and Characterization of Si/Cs/O Nanocluster Thin Films with Negative Electron Affinity, *Physical Review B*, **59**, pp.15513-15522.

[20] Chase L.L., Balooch M., Siekhaus W.J. (1996) Optical Properties of Passivated Si Nanocrystals and SiO_x Nanostructures, *Physical Review B*, **54**, pp.5029-5037.

[21] Tolbert S.H., Herhold A.B., Brus L.E., Alivisatos A.P. (1996) Pressure-Induced Structural Transformations in Si Nanocrystals: surface and shape effects, *Physical Review Letters*, **76**, pp.4384-4387.

[22] Lee T., Liu J., Chen N.-P., Andres R.P., Janes D.B., Reifenberger R. (2000) Electronic Properties of Metallic Nanoclusters on Semiconductor Surfaces: implications for nanoelectronic device applications, *Journal of Nanoparticle Research*, **2**, pp.345-362.

[23] Киттель Ч. (1978) *Введение в физику твердого тела.* Москва: Наука.
Калоджеро Ф. (1978) *Метод фазовых функций в теории потенциального рассеяния.* Москва: Мир.

[24] Shunin Yu.N., Budilov K., Zhukovskii Yu.F., Sychev O., Borstel G. (2003) Electronic and Elastic Pproperties of CU-Interconnectors. In: *Proc. of the 1st Int. Conf. Information Technologies and Management*, pp.99-111.

[25] Слэтер Дж. (1978) *Методы самосогласованного поля для молекул твердого тела.* Москва: Мир.

[26] Gopejenko V.I., Gopejenko A.V., Shunin Yu.N (2004) Methods of Phase Functions in the Electronic Structure Calculations of Disordered Solids. In: *Proc. of the 2nd Int. Conf. Information Technologies and Management,* pp.138-140.

[27] Shunin Yu.N. , Budilov K. (2004) Electron Properties of Silicon-Based Disordered Systems. In: *Proc. of the 2nd Int. Conf. Information Technologies and Management ,* pp.129-137.

[28] Gopeyenko A., Gopeyenko V., Shunin Yu. (2005) Data Base of Nanoclusters Fundamental Electronic and Mechanical Properties Creation. In: *Theses of the 3rd Int. Conf. Information Technologies and Management*, pp.43-44.

Received on the 21st of May 2005

Computer Modelling and New Technologies, 2005, Vol.9, No.1, 32-39
Transport and Telecommunication Institute, Lomonosov 1, LV-1019, Riga, Latvia

MATHEMATICAL MODELLING OF THE WIRELESS COMMUNICATION NETWORK

M. KOPEETSKY

Department of Computer Engineering, Holon Academic Institute of Technology,
Golomb 52, Holon 58102
E-mail: mkopeets@012.net.il , Tel: 972-3-5026531, Fax: 972-3-5026510

The paper is devoted to study and evaluation of the erroneous packets flow on the physical layer of a wireless communication network. A mathematical model of the erroneous packets passed to the communication channel has been structured and analysed. The statistical estimation of the erroneous packets number is presented and discussed in the paper.

Keywords: *Wireless communication channel, erroneous packets, error bursts.*

1. Introduction

Most communication systems are sensitive to random errors and synchronization failures. The Physical Layer analysis of any Computer Communication network is very important. This is because many different problems concerning network execution and utilization are caused by errors and failures on the Physical Layer. Wireless communication networks are not the exception. Moreover, the problem of achieving high reliability and error tolerance is urgent in modern communication technologies such as mobile Internet Protocol (IP) or General Packet Radio Service (GPRS) networks [1].

A number of problems arise in a wireless communication channel context. These problems are caused by the following reasons. The first reason is related to non-reliability of the radio channel. As a matter of fact, a sufficiently high Bit Error Rate (BER) and very high synchronization failure probability as opposed to the qualitative wire and especially fiber optic channels characterize these channels. BER may be rather within $10^{-1} - 10^{-3}$. The second reason is that BER in the radio channel is not a constant value. As soon as the reliability of the wireless channel depends on several external reasons, BER is essentially a time function. However, in recent years there has been an intensive interest in wireless channels. A number of papers devoted to the impact of burst errors on the network reliability and on packet synchronization have appeared [2, 3], among others.

2. General Principles for Determining the Probabilistic Model of the Wireless Channels

A various range of BER within a given Virtual Connection characterizes wireless communication channels. Therefore, it is reasonable to create an appropriate probabilistic model of the wireless channel. The purpose of this paper is to analyse the general number of erroneous packets during a specific time interval. It should be mentioned that BER and Packet Error Rate (PER) do not change during a packet transmission in the presented model. The PER change is expected after the ending of a given packet transmission. Mention that PER is a BER function in a network model.

Let us assume that there is n^* various channel states. Each channel state is defined by a specific PER $\overline{p}$. Actually, $\overline{p}$ is a discrete random variable. For each channel state i, $\overline{p}$ is equal to $\overline{p}_i$. Let's assume that the current channel state corresponding to the given packet transmission is 1. Then $\overline{p} = \overline{p}_1$. For the next packet transmission there exists a finite probability $(1-\gamma_0^{(1)})$ of non- changing of the current channel state 1. Let us denote the probabilities set $\gamma_0^{(2)},...,\gamma_0^{(i)},...\gamma_0^{(n^*)}, (\sum_{i=2}^{n^*}\gamma_0^{(i)} = 1-\gamma_0^{(1)})$.

Each $\gamma_0^{(i)}$ value specifies a probability that within a next packet transmission a channel state will be i.

Actually, a simple Markov chain may describe the discrete process that determines the current channel state [4]. The chain is defined by the probability transition matrix $Z = (z_{ij})$ and by the initial probabilistic

vector $\pi(0)=[10...0]$. Evidently, *dim(Z)=n**. The Markov chain is homogeneous. The homogeneity is caused by the following reasons:

- The packet flow in the communication channel is stationary.
- The packet transmission time is assumed to be finite and constant. It should be remarked that packet transmission time variance and in the packet processing time variance are omitted.

The concise evaluation of the erroneous packets number causes significant difficulties, which are related to the variability of the probability $\overline{p}$. Therefore, the proposed mathematical model is directed to the probabilistic evaluation of the researched characteristics.

3. The Distribution of the Erroneous Packets Number in Case *n*=2*

Assume that a single change of the $\overline{p}$ value is probable during a transmission of several packets (Figure 1).

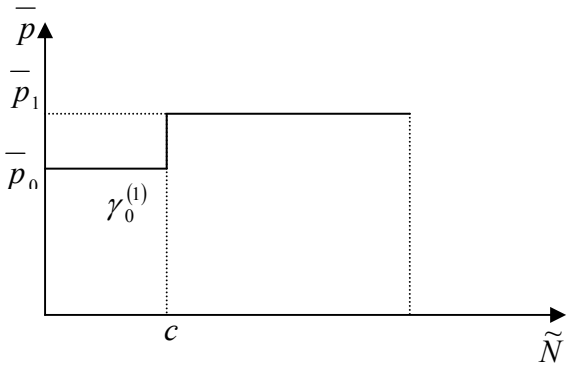


Figure 1. The channel state probability $\overline{p}$ as a function of a transmitted packet number *c* in the case *n*=2.*

The probability of the change of the channel state 1 is equal to $\gamma_0^{(1)}$. It can be assumed that the channel state 1 was changed after a transmission of *(c-1)* packets. Then the previous *(c-1)* packets are characterized by the PER $\overline{p}_0$ while the next *(N-c+1)* cells are characterized by the PER $\overline{p}_1$. The following discrete random variables $y_j^{(1)}$ and $y_j^{(2)}$ are introduced:

$$P\{y_j^1=1\}=\overline{p}_0$$
$$P\{y_j^1=0\}=1-\overline{p}_0$$
$$j=1,...,c-1$$
$$P\{y_j^2=1\}=\overline{p}_1$$
$$P\{y_j^2=0\}=1-\overline{p}_1$$
$$j=c,...N.$$

The discrete random variables $Y_{c-1}^{(1)}=\sum_{j=1}^{c-1}y_j^{(1)}$ and $Y_c^{(2)}=\sum_{j=c}^{N}y_j^{(2)}$ are defined.

Since the random variables under consideration are discrete and integer, it is reasonable to determine the Generating Functions (GF) [4, 5] of the *s* abstract variable:

$$\pi_{Y/c-1}^1(s)=\sum_{x=1}^{c-1}P\{Y_{c-1}^{(1)}=x\}\cdot s^x=[1-\overline{p}_0\cdot(1-s)]^{c-1},\pi_{Y/c-1}^2(s)=$$

$$\sum_{x=1}^{N-c+1}P\{Y_{c-1}^{(2)}=x\}\cdot s^x=[1-\overline{p}_1\cdot(1-s)]^{N-c+1}.$$

Since the random variables $Y_{c-1}^{(1)}$ and $Y_c^{(2)}$ are independent for a fixed value *(c-1)*, then the Generating Function of the random variable $Y_{c-1}=Y_{c-1}^{(1)}+Y_c^{(2)}$ is determined as

$$\pi_{Y/c-1}(s)=\pi_{Y/c-1}^{(1)}(s)\cdot\pi_{Y/c-1}^{(2}(s)=[1-\overline{p}_0\cdot(1-s)]^{c-1}\cdot[1-\overline{p}_1\cdot(1-s)]^{N-c+1}. \quad (1)$$

The random variable Y_{c-1} determines the erroneous packets number under the condition that the channel state was switched on after the *(c-1)* packet transmission. The GF $\pi_{Y/c-1}(s)$ characterizes conditional distribution of the erroneous packets number under the following condition: *c=N-l+1*. Here *l* denotes the number of packets, which have been transmitted in channel state 2. The GF corresponding to the unconditional distribution *Y* is generated as

$$\pi_Y(s)=\sum_{l=1}^{N}\{\pi_{Y/l}(s)\cdot P(l)\}=\sum_{l=1}^{N}\{[1-\overline{p}_0\cdot(1-s)]^{N-l}\cdot[1-\overline{p}_1\cdot(1-s)]^{l}\cdot P(l)\}=$$
$$[1-\overline{p}_0\cdot(1-s)]^{N}\cdot\{P(0)+\frac{1-\overline{p}_1(1-s)}{1-\overline{p}_0(1-s)}\cdot P(1)+\ldots+\left[\frac{1-\overline{p}_1(1-s)}{1-\overline{p}_0(1-s)}\right]^{N}\cdot P(N)\}. \quad (2)$$

P(l) is the random variable *l* distribution [6]. Clearly, the sum from the equation *(2)* is essentially the GF of the random variable *l* with the argument $\frac{1-\overline{p}_1(1-s)}{1-\overline{p}_0(1-s)}$, which substitutes the argument s. Consequently,

$$\pi_Y(s)=[1-\overline{p}_0\cdot(1-s)]^{N}\cdot\pi_l\cdot\left[\frac{1-\overline{p}_1\cdot(1-s)}{1-\overline{p}_0\cdot(1-s)}\right]. \quad (3)$$

The equation *(3)* contains information about $\gamma_0^{(1)}$ by means of the items *P(l)*. The first item of $\pi_Y(s)$ $[1-\overline{p}_0\cdot(1-s)]^{N}$ determines GF of the binomial (Bernoulli) distribution with the argument *s*. Let us take up the limit transition that is investigated if $N\to\infty$. Such situation is relevant if the number of transmitted packets is sufficiently large. For this purpose the following rates are introduced:

$$a_0=\frac{\overline{p}_0}{\gamma_0^{(1)}},a_1=\frac{\overline{p}_1}{\gamma_0^{(1)}},\widetilde{d}=N\cdot\gamma_0^{(1)}.$$

The random variable $\widetilde{Y}$ that is characterized by the binomial distribution with the GF $\pi_{\widetilde{Y}}(s)=[1-\overline{p}_0\cdot(1-s)]^{N}$, is also introduced. The purpose is to determine

$$\lim_{N\to\infty}\pi_{\widetilde{Y}}(s)=\lim_{N\to\infty}[1-a_0\gamma_0^{(1)}\cdot(1-s)]^{N}=e^{-\widetilde{d}a_0(1-s)}.$$

Considering the PER switching mechanism let's find the limit of the second item of the $\pi_Y(s)$. Clearly,

$$P(0)=(1-\gamma_0^{(1)})^{N-1},P(1)=(1-\gamma_0^{(1)})^{N-2}\cdot\gamma_0^{(1)},\ldots,P(N-1)=\gamma_0^{(1)},P(N)=0.$$

Hence,

$$\pi_l\left[\frac{1-\overline{p}_1(1-s)}{1-\overline{p}_0(1-s)}\right]=(1-\gamma_0^{(1)})^{N-1}+\left[\frac{1-\overline{p}_1(1-s)}{1-\overline{p}_0(1-s)}\right]\cdot(1-\gamma_0^{(1)})^{N-2}\cdot\gamma_0^{(1)}+\cdots+\left[\frac{1-\overline{p}_1(1-s)}{1-\overline{p}_0(1-s)}\right]^{N-1}\cdot\gamma_0^{(1)}=$$
$$\gamma_0^{(1)}(1-\gamma_0^{(1)})^{N-2}\cdot\left[\frac{1-\overline{p}_1(1-s)}{1-\overline{p}_0(1-s)}\right]\cdot\frac{1-\left\{\frac{1-\overline{p}_1(1-s)}{1-\overline{p}_0(1-s)(1-\gamma_0^{(1)})}\right\}^{N-1}}{1-\frac{1-\overline{p}_1(1-s)}{1-\overline{p}_0(1-s)(1-\gamma_0^{(1)})}}++(1-\gamma_0^{(1)})^{N-1}. \quad (4)$$

By carrying out all actions related to the determining of the $\lim\pi_l\left(\frac{1-\overline{p}_1(1-s)}{1-\overline{p}_0(1-s)}\right)$, we conclude that

$$\pi_Y^0(s)=\lim_{N\to\infty}\pi_Y(s)=e^{-\widetilde{d}a_0(1-s)}\cdot\left[e^{-\widetilde{d}}+\frac{e^{-\widetilde{d}v(1-s)}-e^{-\widetilde{d}}}{1-v+vs}\right], \quad (5)$$

where $v=a_1-a_0$.

In summary, any order initial distribution moment of the random variable under consideration is determined on the $\pi_Y^0(s)$ base. As a matter of fact, exact determination of the erroneous packets number is possible if *n=2* and the only single switch of the channel mode is probable.

4. Analysis of the Erroneous Packets Number in Case *n*>2*

In a general case, if during a specific interval *S,* the number of channel modes switches is more than one, as well as in the case *n**=3, the distinct calculation of $\pi_Y^0(s)$ is rather complicated. The problem discussion is presented for *n**=3. It can be assumed that the channel switching procedure is depicted in Figure 2.

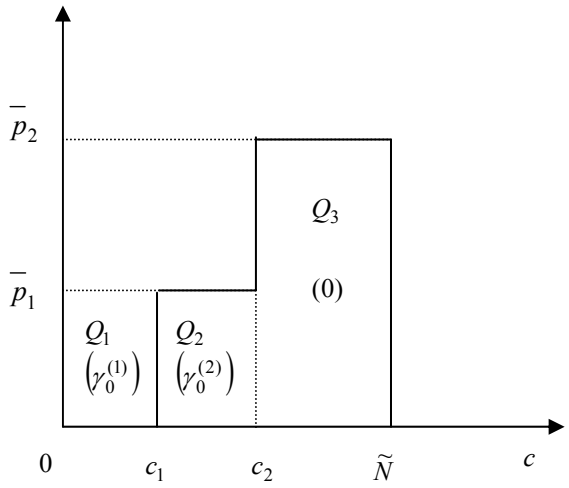


Figure 2. The channel state probability $\overline{p}$ as a function of a transmitted cell number *c* in case *n*=3.*

The following assumptions are made:

1. The only two leaps of the probability $\overline{p}$ are possible during a specific time interval *S.*
2. On the first stage, $\overline{p}=0$. It means that no error takes place during the transmission of *(c-1)* packets.
3. The two channel state switches are possible with the probabilities $\overline{p}_1$ and $\overline{p}_2$ after the transmission of (c_1-1) and (c_2-1) packets respectively.

As a result the graph $\overline{p}(c)$ includes the tree areas: Q_1, Q_2 and Q_3. The channel state switch probability in the area Q_1 or Q_2 is γ_0^1 or γ_0^2 consequently. In the area Q_3 this probability is equal to *0*. The random variables $y_j^{(1)}$ and $y_j^{(2)}$ are defined as in the previous case. Then

$$\pi_Y(s)=\pi_l\cdot[1-\overline{p}_1\cdot(1-s)]\ \cdot(1-\gamma_0^2)+$$
$$+\frac{\gamma_0^2\cdot\dfrac{1-\overline{p}_2(1-s)}{1-\overline{p}_1\cdot(1-s)}}{\dfrac{1-\overline{p}_2(1-s)}{1-\overline{p}_1\cdot(1-s)}+\gamma_0^2-1}(\pi_l[1-\overline{p}_2(1-s)]-\pi_l[1-\overline{p}_1(1-s)]\cdot(1-\gamma_0^2))). \qquad (6)$$

According to the assumption, no packet error is possible in the range *[1,…,c-1*]. The arguments of the GFs $\pi_l\{f(s)\}$ essentially are the functions of *s*. Therefore $\pi_l\{f(s)\}$ are formed from *(4)* by means of the argument changing of $\dfrac{1-\overline{p}_2\cdot(1-s)}{1-\overline{p}_1\cdot(1-s)}\to f(s)$. Clearly, the dependence $\pi_Y(s)$ on γ_0^1 is reflected in the argument change. Such dependence is absent in *(6)* in the obvious form. The considerable calculation difficulties arise during a limit transition when $N\to\infty$. The function $\pi_Y^0(s)$ as well as in the previous case contains the item $e^{-\tilde{d}}$. Contrary to the previous model, $\pi_Y^0(s)$ is not represented as the multiplication of the GFs number. However, this problem can be solved by means of numerical methods based on the computer calculations.

The presented Table 1 demonstrates the mathematical expectation and variance of the erroneous packets number *Y* considering the parameters $\overline{p}_1, \overline{p}_2, \gamma_0^1, \gamma_0^2, N$.

TABLE 1. Mathematical expectation E_Y and variance V_Y of the non-synchronous cells number *Y*. *N*=10.

$\overline{p}_1$	$\overline{p}_2$	γ_0^1	γ_0^2	E_Y	V_Y
10^{-8}	10^{-6}	10^{-1}	10^{-1}	$1.2 \cdot 10^{-7}$	$8.5 \cdot 10^{-10}$
10^{-8}	10^{-6}	0.2	10^{-1}	$8.9 \cdot 10^{-6}$	$4.5 \cdot 10^{-8}$
10^{-8}	10^{-6}	0.8	10^{-1}	$1.3 \cdot 10^{-5}$	$2.0 \cdot 10^{-8}$

5. Evaluation of the Erroneous Packets Number in Case of any *n** and $N \to \infty$

It should be stated that in a more general case it is not reasonable to study the erroneous packets number by means of the discrete distributions. Therefore, the transition from the discrete random variable to the continuous one is required. Hence, study of the discrete random variable *Y* distribution is replaced by the evaluation of the continuous random variable *U* distribution moments. The researched characteristic *U* takes all possible values in the range $[0, N]$. Moreover, the *Y* and *U* mathematical expectations are equal: $E^Y = E^U$. It should be assumed that the transition condition of the Central Limit Theorem takes place, i.e. E^U, is sufficiently large.

According to the general principles of the research methods of continuous random variables, The Moment Generating Function (MGF) is introduced $M_U(\eta) = \int_{-\infty}^{+\infty} e^{U\eta} \cdot \varphi(U) dU$, where $\varphi(U)$ is the probability density of the random variable *U*. Evidently, GFs and MGFs are connected by common features. Analyzing the problem under consideration $M_U(\eta)$ is formed from $\pi_{\widetilde{Y}}(s)$ (or $\pi_Y^0(s)$) by the argument change $s \to e^{\eta}$. Consequently, based on the theorem of continuity and on the theorem of uniqueness [1], the limit $M = \lim_{\eta \to \infty} M_U(\eta)$ defines the *U* limit distribution function (or probability density function) in the unique way if $N \to \infty$. The general theorem of continuity sets correspondence between the limit distribution functions and the MGFs of a certain argument. As a matter of fact, in the continuous distribution case, any initial or central *U* distribution moment of the *j-th* order is not equal to the corresponding moment of the *Y* discrete distribution if $N \to \infty$. However, the following inequality is correct:

$$\mu_j^U \le \mu_j^Y, j \ge 2. \tag{7}$$

Actually this inequality is caused by the following reasons: in the general case of the *U* continuous distribution for the analysis of the $\widetilde{p}(c)$ function not a single realization with a given probability, but the random variable *w* distribution must be taken into account. Actually, *w* takes w_m values that denote the channel switch from the current state to the *m* state for the next packet transmission (Figure 3). Obviously, the normalizing condition takes place: $\sum_{m=1}^{n^*} P(w_m) = 1$.

The proposed mathematical method is based on the change of all random process realizations that correspond to the channel state *b* switch to the set of the other possible channel states, by the average realization. This realization is specified by the channel state switch probability $\widetilde{p}_b = \sum_{m \ne b}^{n^*} \widetilde{g}_m \cdot \widetilde{p}_m$, where $\widetilde{g}_m$ is the average probability of the channel state *m*. This fact immediately explains the inequality (7).

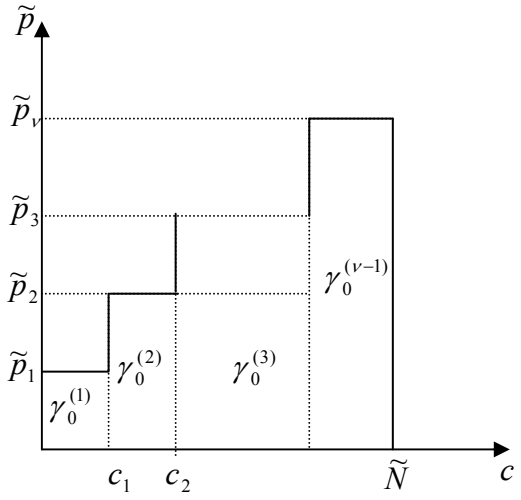


Figure 3. The channel state probability $\overline{p}$ as a function of a transmitted packet number *c* in the case of any *n**

The case of *n*=2* will be discussed further. The transition from $\pi_Y^0(s)$ *(5)* to the corresponding MGF is executed by means of argument change $s \to e^{\eta}$:

$$M_U(\eta) = e^{-\widetilde{d}a_0(1-e^{\eta})} \cdot \left[e^{-\widetilde{d}} + \frac{e^{-\widetilde{d}v(1-e^{\eta})-e^{-\widetilde{d}}}}{1-v+vs} \right]. \tag{8}$$

Assuming that $\widetilde{p}_0$ is rather small, the first item tends to 1. Each *j-th* order initial distribution moment is derived by means of the *j-th* order derivative in the point $\eta = 0$. Hence the generated distribution function determines the low limit of any order initial (or central) distribution moment. In order to study the more general dependence $\widetilde{p}(c)$ (Figure 3) the following limitations are introduced: $\widetilde{d} \to \infty, a_1 \to \infty$ (conditions $*$). The first condition $(\widetilde{d} \to \infty)$ takes place in the case when the channel state switch (or switches) occurs with a sufficiently high probability if the cells transmission time is rather large. The second condition $(a_1 \to \infty)$ covers the case when the channel switches are rather rare. Then the random variable *U* is transformed into the random variable *B* such as $M_B(\eta) = \lim_{\widetilde{d}, a_1 \to \infty} M_U(\eta)$. Based on the solution methods of the analogous problems in Probability Theory in relation to the continuous distributions [5], the *B* random variable is represented as the linear combination of the independent random variables B_l. The B_l number depends upon the $\widetilde{p}(c)$ jumps. In fact for the model represented by Figure 2 the following equation is correct: $B = B_1 - \frac{1}{2}a_1 B_2$. It is assumed that the packet error in the channel state 1 is impossible. Here the B_1 random variable follows the normal distribution with the mathematical expectation and the variance $E(B_1) = V(B_1) = a_1\widetilde{d}$. The B_2 random variable also follows the χ^2-distribution with two degrees of freedom, i. e., the B_2 probability density function is $\varphi(B_2) = \frac{1}{2}e^{-\beta_2/2}$. In the same way in the case *n*=3* from the previous paragraph $B = B_1 - \frac{1}{2}a_2 B_2 - \frac{1}{2}(a_2 - a_1)\Delta_1 B_3$. Here $\Delta_1 = \frac{\gamma_0^1}{\gamma_0^2}, a_2 = \frac{\widetilde{p}_2}{\gamma_0^1}$.

B_1 is characterized by a normal distribution with the parameters $E(B_1) = V(B_1) = a_2\widetilde{d}$. Finally, B_2 and B_3 follow the χ^2 – distribution with two degrees of freedom. Analogously in the general case (Figure 3) the *Y* random variable is transformed into the continuous random variable *B* under the limit transition:

$$B = B_1 - \frac{1}{2}a_\upsilon B_2 - \frac{1}{2}(a_\upsilon - a_1)\Delta_1 B_3 - \cdots - \frac{1}{2}(a_\upsilon - a_{\upsilon-1})\Delta_{\upsilon-1}B_{\upsilon+1}. \quad (9)$$

Here B_1 is characterized by the normal distribution with the parameters

$$E(B_1) = V(B_1) = a_\upsilon\widetilde{d}, a_f = \frac{\widetilde{p}_f}{\gamma_0^1}, \Delta_f = \frac{\gamma_0^1}{\gamma_0^f}.$$

Consequently, the MGF of the erroneous packets number, which is approximated by the random variable *B*, is determined as the MGF items multiplication. Indeed the *B* items distributions are known. If all items in *(9)* are of the close orders, then the *B* distribution tends to the normal distribution. This fact is confirmed by the Lapunov theorem:

Assuming that the random variable *z* is presented as $z = z_1 + z_2 \ldots + z_k$, where $z = z_1, z_2, \ldots, z_k$ are the independent random variables and *k* growth is unlimited. The random variable z_k distribution function is

$$F_k(z) = \int_{-\infty}^{z} f(z)dz.$$

If $\lim\limits_{k\to\infty} \frac{\sum_{i=1}^{k} E(z_i - E(z_i))^3}{(V(z))^{3/2}} = 0$, (**)

then $\lim\limits_{k\to\infty} F_k(z) = \Phi\left(\frac{z - E(z)}{V(z)}\right)$.

Here $\Phi(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{t} e^{\frac{-y^2}{2}} dy$ is the Laplace function. Therefore, if the limit (**) takes place and the number of *k* items is sufficiently large, then the *z* random variable distribution is closed to the normal distribution. Otherwise, if among the items $(a_\upsilon - a_f)\Delta_f$ there are items greatly different from the others, then the *B* random variable is approximated by the sum [6]: $B = B_1 + hB_2, h = const$. Each initial *B j-th* order distribution moment μ_j^B is calculated as $\mu_j^B = \left(\frac{d^j}{ds} M_B(s)\right)_{s=0}$. Finally, μ_j^B is substituted by the μ_r^U evaluation in the inequalities (7).

Conclusions

The following remarks complete the paper.

- It is possible to create the similar mathematical model in the case when packet errors are not neglected in the range $[0, c_1]$. The above mentioned range corresponds to the $\gamma_0^{(1)}$ probability.
- The monotonous growth of the $\overline{p}$ and $\widetilde{p}$ values by the transmitted packets number increment is assumed. Nevertheless, this assumption is not necessary. Moreover, there are no limitations on the $\overline{p}(c)$ or $\widetilde{p}(c)$ functions jumps if the conditions $(*)$ take place. Actually, based on equation (9) in the non-monotonous $\widetilde{p}(c)$ case the $\widetilde{p}_\upsilon$ is equal to the maximal $\widetilde{p}_f$ probability.
- It should be mentioned that $\widetilde{p}_f$ value corresponds to a given channel state switch. Evidently, the items order in the sum is meaningless.
- Finally, the limit transition $N \to \infty$ is legitimate if the transmitted cells number is sufficiently large. Several problems are considered for future work. Based on the real data, the modified decoding algorithm that appropriates to the non-reliable noisy wireless environment should be chosen and applied in the modern mobile IP or GPRS technologies. Thus, the PER in the wireless network should be decreased. Consequently, the network reliability should be significantly improved in comparison with the existing models.

References

[1] Kurose J., Ross K. (2003) *Computer Networking. A Top Down Approach Featuring the Internet,* 2nd ed. Addison Wesley.
[2] Yang L., Xiaokang L., Kewu P. (1999) Cell Synchronization Under a Special Error Protection Mechanism. In: *Fifth Asia-Pacific Conference on Communications and Fourth Optoelectronics and Communications Conference (China)*, Vol. 1, pp. 109-106.
[3] Zorzi M. (1999) On the Impact of Burst Errors on Wireless ATM, *IEEE Personal Communications*, pp.65-76.
[4] Papoulis A. (1991) *Probability, Random Variables, and Stochastic Processes,* 3rd ed. McGraw-Hill.
[5] Duduvicz E. J., Mishra S. N. (1998) *Modern Mathematical Statistics*. New York: Wiley.
[6] Kordonsky X. (1963) *Application of Probability Theory for Engineers*. Moscow: State Publishing of the Mathematical and Physical Literature.

Received on the 21st of May 2005

Computer Modelling and New Technologies, 2005, Vol.9, No.1, 40-46
Transport and Telecommunication Institute, Lomonosov 1, LV-1019, Riga, Latvia

ALTERNATIVE STOCHASTIC NETWORK PROJECTS WITH RENEWABLE RESOURCES

Z. LASLO[a], D. GOLENKO-GINZBURG[b,c], A. GONIK[c]

[a] *Department of Industrial Engineering and Management, Sami Shamoon College of Engineering, Beer Sheva, 84100, Israel, E-Mail: zohar@sce.ac.il*
[b] *Department of Industrial Engineering and Management, Academic College of Judea and Samaria, Ariel, 44837, Israel*
[c] *Department of Industrial Engineering and Management, Ben-Gurion University of the Negev, Beer Sheva, 84105, Israel*

The paper presents a heuristic for resource constrained network project scheduling. A network project comprising both alternative deterministic decision nodes and alternative branching nodes with probabilistic outcomes is considered. Several renewable activities related resources, such as machines and manpower, are imbedded in the model. Each type of resources is in limited supply with a resource limit that is fixed at the same level throughout the project duration. Each activity in the project requires resources of various types with fixed capacities. The activity duration is a random variable with given density function. The problem is to minimize the expected project duration by determining for each activity, which will be realized within the project's realization, its starting time (decision variable), i.e., the time of feeding-in resources. The resource delivery schedule is not calculated in advance and is based on decision-making in the course of monitoring the project. The suggested heuristic algorithm is performed in real time via simulation. Decision-making is carried out:

- at alternative deterministic decision nodes, to single out all the alternative subnetworks (joint variants) in order to choose the one with the minimal average duration;
- at other essential moments when at least one activity is ready to be operated but the available amount of resources is limited. A competition among those activities is carried out to determine the subset of activities which have to be operated first and can be supplied by available resources. Such a competition is realized by a combination of a knapsack resource reallocation model and a subsidiary simulation algorithm.

Keywords: *Alternative decision nodes, probabilistic branching, joint variant, renewable resources, resource constrained GERT project scheduling algorithm, stochastic project simulation*

1. Introduction

While the literature on PERT and CPM network techniques is quite vast, the number of publications on *alternative networks* remains very scanty. Various authors, e.g. Eisner [4], Elmaghraby [6], Pristker [17], Whitehouse [19], etc., introduced the concept of a research and development (R&D) project as a complex of actions and problems towards achieving a definite goal. Several adequate network models for such projects have been considered. The first significant development in that area was the pioneering work of Eisner [4] in which a "decision box" with both random and deterministic alternative outcomes was introduced. Elmaghraby [5, 6] introduced additional logic and algebra in network techniques, while Pritsker, Happ and Whitehouse [15, 16] developed the GERT techniques for alternative network models with stochastic outcomes in key nodes. Xespos and Strassman [20] introduced the concept of the stochastic decision tree, while Crowston and Thompson [1-3] and later on Hastings and Mello [12] introduced the concept of multiple choices at such alternative nodes, when decision-making is of a deterministic nature (Decision-CPM models). Lee, Moeller and Digman [13-14] developed the VERT model that enables the analyst to simulate various decisions with alternative technology choices within the stochastic decision tree network. Golenko-Ginzburg [7] has developed a unified controlled alternative activity network (CAAN model) for projects with both random and deterministic alternative outcomes in key nodes. At each routine decision-making node, the developed algorithm singles out all the subnetworks (the so-called joint variants) that correspond to all possible outcomes from that node. Decision-making results in determining the optimal joint variant and following the optimal direction up to the next decision-making node. However, the techniques thus far developed can only be applied to fully divisible networks that can be subdivided into non-intersecting fragments. The CAAN model does not include non-fully-divisible networks. Thus, the model is not relevant to most R&D projects, since the latter are usually structured from non-divisible subnetworks. Golenko-Ginzburg and Blokh [8] have developed a more universal alternative network – the Generalized Alternative

Activity Network (GAAN model). All types of the previously developed alternative network models, namely, Eisner's model, GERT, Decision-CPM, VERT and CAAN networks, are particular cases of the GAAN model. In recent years a SATM alternative network model has been described [18]. However, despite the GAAN model, the SATM model does not comprise algorithms to be optimised.

2. Model's description

A GAAN model is a finite, oriented, acyclic activity-on-arc network $G(N, A)$ with the following properties:

I. $G(N, A)$ has one source node n_0 and no less than two sink nodes n'.

II. Each activity $(i, j) \in A$ refers to one of three different types as follows:

Type 1 activity (i, j) is a PERT activity (PA) with the logical "must follow" emitter at node i and the "and" receiver at node j;

Type 2 activity (i, j) is an alternative stochastic activity (ASA) with the logical "exclusive or" emitter at node i. Each $(i, j) \in A$ of ASA type corresponds to probability $o < p_{ij} < 1$, while node i comprises a set of not less than two probabilities p_{ij}, $\sum_j p_{ij} = 1$;

Type 3 activity (i, j) is an alternative deterministic activity (ADA) with the logical "exclusive or" emitter at node i. Node i is a decision-making node and the corresponding transfer probabilities sum to one.

III. Activities of all types may leave one and the same node. Thus, unlike the CAAN model, the GAAN model is not a fully divisible network.

IV. Activities of all types may enter one and the same node.

An example of the GAAN model is presented in Figure 1.

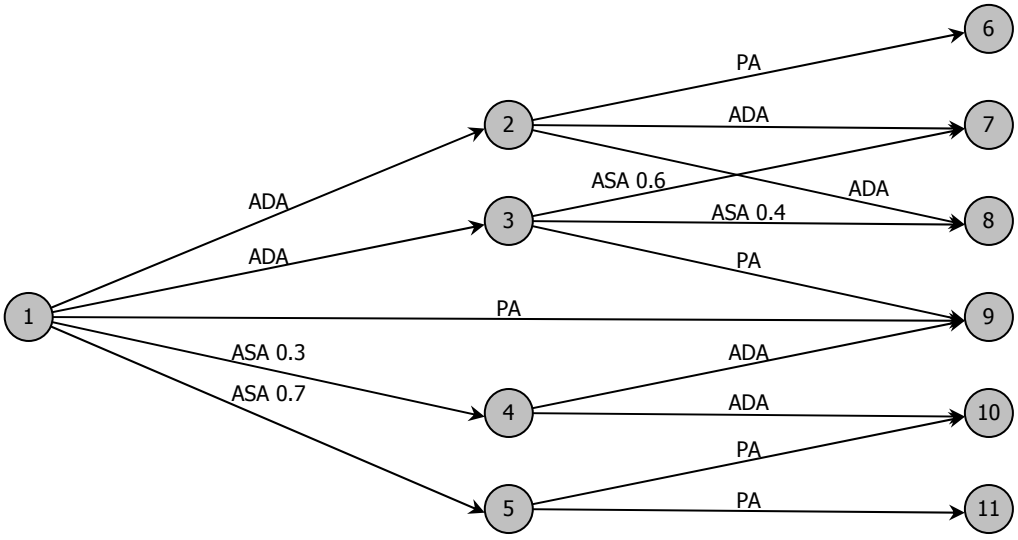


Figure 1. The GAAN type graph

We will call *a joint variant of the GAAN model* $G(N, A)$ a subgraph (subnetwork) $G^*(N^*, A^*)$ satisfying the following conditions:

1. $G^*(N^*, A^*)$ has one source node;
2. If $G^*(N^*, A^*)$ comprises a certain node i, i.e., $i \in N^*$, then $G^*(N^*, A^*)$ comprises all activities (i, j) of type PA and ASA leaving node i;
3. If $G^*(N^*, A^*)$ comprises a certain node i which in the GAAN model $G(N, A)$ has alternative outcomes of ADA type then $G^*(N^*, A^*)$ comprises only one activity of that type leaving that node;

4. $G^*(N^*, A^*)$ is the maximal subgraph satisfying conditions 1-3.

Call *a full variant of the joint variant* $G^*(N^*, A^*)$ a subnetwork of PERT type $G^{**}(N^{**}, A^{**}) \subset G^*(N^*, A^*)$, which can be extracted from the latter by simulating non-contradicting outcomes of ASA type in interconnected nodes and excluding alternative non-simulated outcomes.

Call *a probability of realizing a full variant* G^{**} a product of all values p_{ij} for all activities of ASA type entering the full variant.

3. Decision-making in GAAN models

To control a project, such as any production process, it is necessary to introduce decision-making in order to reach the goal while optimising a given objective (the optimal value OV) subject to certain restrictions (the restrictive values RV). When the objective is the project's duration, the first restriction is usually a resource restriction and vice-versa. For a project represented by a GAAN type model decision-making means choosing the directions of the project's progress in controlled nodes (decision-making nodes) with alternative outcomes of ADA type, since alternatives of ASA type are uncontrollable. Thus, the optimisation problem consists of the following steps:

STEP 1. At each decision-making node which has been reached at moment t in the course of the project's realization:
- to determine and to single out all the joint variants from the remaining project G_t at moment t;
- to calculate the optimised value OV and all the restrictive values RV for each variant.

STEP 2. To determine the optimal joint variant and to follow the optimal direction up to the nearest decision-making node. The problem must be repeatedly solved for the reduced network in every sequentially encountered decision-making node.

4. The optimal problem

The mathematical formulation of the problem is as follows: determine the optimal joint variant $G^{*opt} \subset G(N, A)$ that optimises the objective function:

$$E[F(G^{*opt})] = \underset{\{G^*\}}{\text{Min(Max)}} \sum_{\{G^{**}\} \subset G^*} [F(G^{**}) \cdot \Pr\{G^{**}\}], \quad (1)$$

s.t.

$$E[Q_\nu(G^{*opt})] = \sum_{\{G^{**}\} \subset G^*} [Q_\nu(G^{**}) \cdot \Pr\{G^{**}\}] \le H_\nu, \qquad 1 \le \nu \le V. \quad (2)$$

Here $F(G^{**})$ is the objective function of full variant G^{**}, $\Pr\{G^{**}\}$ is the probability of realizing G^{**}, $Q_\nu(G^{**})$ is the value of the ν-th restricted criterion and H_ν is the pre-set restriction level for that criterion. Note that for certain particular cases V may be zero, i.e., the optimal problem has no restrictions, or the problem comprises only one restriction (2) without objective (1). *Since problem (1-2) is NP-complete* [8] *in order to obtain an optimal solution one has to develop a look-over algorithm to single out all the joint variants*.

The idea to enumerate the joint variants of the CAAN model [7] is based on introducing the lexicographical order to the set of maximal paths in the CAAN graph. The corresponding look-over algorithm is very simple in usage [7]. In the case of a GAAN network the order on the set of paths has to be substituted for the order on the set of subgraphs [8]. To develop the enumeration algorithm, we use the ideas to enumerate the so-called trajectories for assignment problems, or special matrices for travelling salesman problems [8, 10]. Note that singling out the maximal trajectory for an assignment problem is similar to determining the joint variant with the maximal objective value. Since a trajectory can be regarded as a vector and the latter, in turn, can be mapped onto a set of integer numbers, the trajectories can be enumerated. Similar ideas are used in developing a look-over algorithm to enumerate and single out all the joint variants.

For the problem under consideration we will use renewable, i.e., non-consumable resources of different types. In some cases resources can be gauged by a single measure, e.g., by the number of standard identical building teams for construction projects [9-11]. Thus, usually objective (1) is the

average joint variant's duration (to be minimized), while restrictions H_ν are pre-given restrictions of the ν-th type renewal resource capacities which are at the disposal of the project's management.

Thus, the problem obtains a two-stage solution as follows:

STAGE 1. To single out the entire joint variant by means of lexicographical order according to the algorithms outlined in [8].

STAGE 2. For each joint variant determine the average value of the project's duration subject to the restricted renewable resource capacities. Stage 2 can be realized via algorithms outlined below. Not that for the case of a fully divisible PERT type joint variant the problem has been solved in [9, 10]. However, in our case the joint variant is a not fully divisible GERT model with stochastic branching ASA and PERT activities PA. We suggest an extension of the quasi-optimal heuristics outlined in [9, 10].

5. Determining the joint variant's average duration

In order to realize Stage 2 we have to implement terms as follows:

- $G^*(N^*, A^*)$ - stochastic network (joint variant) of GERT type;
- $(i, j) \subset A^*$ - the network's activity;
- t_{ij} - random duration of activity (i, j);
- a_{ij} - lower bound of value t_{ij} (pre-given);
- b_{ij} - upper bound of value t_{ij} (pre-given);
- μ_{ij} - average value of t_{ij};
- R_{ijk} - capacity of the k-th type resource(s) allocated to activity (i, j), $1 \le k \le n$ (fixed and pre-given);
- n - number of different resources;
- R_k - total available resources of type k at the project's management disposal (pre-given and fixed throughout the planning horizon);
- $R_k(t) \le R_k$ - free available resources at moment $t \ge 0$;
- S_{ij} - the time that resources r_{ijk} are fed in and activity (i, j) starts (a random value conditional on our decision);
- $T(G^* \mid S_{ij})$ - random project's duration, on condition that feeding-in resources r_{ijk} is carried out at moments S_{ij};
- $R'_k(t \mid S_{ij})$ - maximal value of the k-th resource profile at moment t on condition that activities $(i, j) \subset G(N, A)$ start at moment S_{ij};
- F_{ij} - the actual moment activity (i, j) is finished $(= S_{ij} + t_{ij})$;
- $T(i)$ - earliest possible time of realization node i;
- $p(i, j)$ - conditional probability of activity (i, j) to be on the critical path in the course of the project's realization (dependent on the decisions already taken).

Note that practically all project's activities (i, j) are based on the assumption that each activity duration follows a beta probability density function. We shall henceforth use a beta-distribution as follows:

$$f_{ij}(x) = \frac{12}{(b_{ij} - a_{ij})^4}(x - a_{ij})(b_{ij} - x)^2 . \qquad (3)$$

Besides beta distribution, the model developed may adopt other distributions. Three alternative distributions have been considered in [9, 11]:

1. t_{ij} has a beta distribution with density function (3) in the interval $[a_{ij}, b_{ij}]$;
2. t_{ij} has a uniform distribution in the same interval;

3. t_{ij} has a normal distribution with the mean $\mu_{ij} = 0.5(a_{ij} + b_{ij})$ and the variance $V_{ij} = [(b_{ij} - a_{ij})/6]^2$.

The initial data of the model for each activity (i, j) includes: i; j; a_{ij}; b_{ij}; $r_{ij1},...,r_{ijn}$.

It goes without saying that relations

$$\underset{i,j}{\text{Max}}\, r_{ijk} \le R_k, \qquad 1 \le k \le n, \tag{4}$$

hold, otherwise the project cannot be operated.

6. The simulation model with the Knapsack problem

On the basis of the outlined above notations, we suggest to realize Stage 2 of problem (1-2) via a newly developed step-wise heuristic, as follows:

STEP 1. In all stochastic branching nodes simulate by means of Monte Carlo the outcome activities. Thus, the GERT model after simulation undergoes modification to a PERT model. Call this PERT model $\bar{G}(\bar{N}, \bar{A})$;

STEP 2. For the PERT model obtained at Step 1 the following optimal problem is solved:
determine values S_{ij} for all $(i, j) \subset \bar{G}(\bar{N}, \bar{A})$ to minimize the average duration of $T(\bar{G} \mid S_{ij})$, i.e.,

$$\underset{S_{ij}}{\text{Min}}\, E\{T(\bar{G} \mid S_{ij})\} \tag{5}$$

s.t

$$R'_k(t \mid S_{ij}) \le R_k, \qquad \forall t \ge 0, \qquad 1 \le k \le n. \tag{6}$$

Model (5)-(6) is a stochastic optimisation problem, which cannot be solved, in the general case; the problem only allows a heuristic solution. The basic idea of the heuristic solution is as follows. Decision-making, i.e., determining values S_{ij}, is carried out at essential moments F_{ij} and $T(i)$ (decision points), either when one of the activities (i, j) is finished and additional resources r_{ijk}, $1 \le k \le n$, become available, or when all activities (i, j) leaving node i are ready to be processed. If one or more activities $(i_1, j_1),...,(i_m, j_m)$, $m \ge 1$, are ready to be processed at moment t and all of them can be supplied by available resources, the needed resources are fed in and activities (i_q, j_q), $1 \le q \le m$, begin to be operated at moment t, i.e., $S_{i_q j_q} = t$, $1 \le q \le m$. If, at least for one type k of resources, relation $\sum_{q=1}^{m} r_{i_q j_q k} > R_k(t)$ holds, i.e., there is a lack of available resources at moment t, a competition among the activities has to be arranged to choose a subset of activities that will start to be operated at moment t and can be supplied by resources. Note that problem (5)-(6) is an optimal decision-making model to minimize the expected project duration. Thus, supplying the chosen activities with available resources at each decision point centres on reducing the remaining project's duration as much as possible. This means, in turn, that to carry out the competition the project management has to choose and to operate first the subset of activities that provides the maximal total contribution to the expected project's duration.
The stepwise subalgorithm to undertake such a competition enters the step 2. The subalgorithm comprises the following substeps:

SUBSTEP 2.1. Via simulation determine the probabilities $p(i, j)$ of all activities $(i, j) \subset \bar{G}(\bar{N}, \bar{A})$ to be on the critical path [9];

SUBSTEP 2.2. For each essential moment t determine values $p(i_q, j_q)$, $1 \le q \le m$, for all competitive activities at moment t;

SUBSTEP 2.3 Solve the zero-one programming problem which can be formulated as follows: determine integer values $t_{i_q j_q}$, $1 \le q \le m$, to maximize the objective

$$\underset{\{t_{i_q j_q}\}}{\text{Max}}\{\sum_{q=1}^{m}[t_{i_q j_q} \cdot p(i_q, j_q) \cdot \mu_{i_q j_q}]\} \tag{7}$$

s,t.

$$\sum_{q=1}^{m}(t_{i_q, j_q} \cdot r_{i_q j_q k}) \le R_k(t), \qquad 1 \le k \le n, \tag{8}$$

where $t_{i_q j_q} = \begin{cases} 0 & \text{if activity } (i_q, j_q) \text{ will not obtain resources;} \\ 1 & \text{otherwise.} \end{cases}$

SUBSTEP 2.4. After feeding – in resources for the chosen activities, the next earliest "essential" moment is determined and the project's realization proceeds until the sink node cannot be reached. The corresponding heuristic algorithm to schedule the project is outlined in [9], via simulation model for project $\bar{G}(\bar{N}, \bar{A})$.

SUBSTEP 2.5. Calculate the project's duration $T^w(\bar{G} \mid S_{ij})$, where w is the current number of the simulation run.

SUBSTEP 2.6. Undertake substeps 2.1-2.5 M_1 times in order to obtain representative statistics.

SUBSTEP 2.7. Calculate the average project's $\bar{G}(\bar{N}, \bar{A})$ duration

$$E\{T(\bar{G}, S_{ij})\} = \frac{1}{M_1}\sum_{w=1}^{M_1}\{T^w(\bar{G}, S_{ij})\}. \tag{9}$$

Go to step 1.

STEP 3. Undertake numerous realizations (M_2 times) of Step 2 in order to obtain representative statistics.

STEP 4. Calculate the average time duration of the current joint variant $G^*(N^*, A^*)$

$$E\{T(G^* \mid S_{ij})\} = \frac{1}{M_1 \cdot M_2}\sum_{z=1}^{M_2}\sum_{w=1}^{M_1}\{T^w(\bar{G}^z, S_{ij})\}, \tag{10}$$

where $\bar{G}^z$ is the z-th enumerated joint variant G^{*z} entering the GAAN model $G(N, A)$. After simulation at Step 1 network G^{*z} is reduced to the PERT network $\bar{G}^z$.

STEP 5. Compare all values (10) calculated for each joint variant G^* obtained at Stage 1. The joint variant G^{*t}, which corresponds to the minimal value, is taken as the optimal joint variant G^{*opt}.

Thus, steps 1-5 enable the algorithm to look over all the joint variants and, thus, to solve problem (1-2).

Conclusions

- The heuristic algorithm presented here has been successfully used for monitoring complicated medium-size projects with alternative structure and topology, and with limited activity related renewable resources.
- The developed resource constrained project scheduling algorithm is based on multiple realization of a standardized resource constrained algorithm for GERT models. Such a basic algorithm is easy to implement on a PC. The algorithm can be used for any probability distribution of activity durations.
- The algorithm is performed in real time and adopts a wide range of revisions, alterations, etc., over time, in the course of the project's realization.

Acknowledgment

This research has been partially supported by the Paul Ivanier Center for Robotics Research and Production Management, Ben-Gurion University of the Negev.

References

[1] Crowston W B. and Thompson G. L. (1967) Decision CPM: a method for simultaneous planning, *Operations Research,* **15**, pp.407-426.
[2] Crowston W.B. (1970) Decision CPM: network reduction and solution, *Operations Research,* **21**, pp.435-445.
[3] Crowston W.B. (1971) Models for Project Management, *Sloan Management Review,* **12**, pp.25-42.
[4] Eisner H. (1962) A Generalized Network Approach to the Planning and Scheduling of a Research Project, *Operations Research,* **10**(1), pp.115-125.
[5] Elmaghraby S.E. (1964) Algebra for the Analysis of Generalized Activity Networks, *Management Science,* **10**, pp.494-514.
[6] Elmaghraby S.E. (1977) *Activity Networks: Project Planning and Control by Network Models.* New York: John Wiley.
[7] Golenko-Ginzburg D. (1988) Controlled Alternative Activity Networks in Project Management, *European Journal of Operations Research,* **7**, pp.336-346.
[8] Golenko-Ginzburg D. and Blokh D. (1997) A Generalized Activity Network Model, *Journal of Operation Research Society,* **48**, pp.391-400.
[9] Golenko-Ginzburg D. and Gonik A. (1997) Resource Constrained Project Scheduling with Non-Consumable Limited Resources, *International Journal of Production Economics*, **48**, pp29-37.
[10] Golenko-Ginzburg D. and Gonik A. (1997) Project Planning and Control by Stochastic Network Models. **In:** *Managing and Modelling Complex Projects* /Edited by T. M. Williams. The Netherlands: Kluwer Academic Publishers.
[11] Gonik A. (1995) *Planning and Controlling R&D Stochastic Projects*: a Ph.D. Thesis. Ben-Gurion University of the Negev, Beer-Sheva, Israel.
[12] Hastings M.A., and Mello J.M. (1979) *Decision Networks*. New York: John Wiley.
[13] Lee S.M., Moeller G.L. and Digman L.A. (1981) *Network Analysis for Management Decisions.* Kluwer-Nijhoff, Boston.
[14] Moeller G. L. and Digman L.A. (1981) Operations planning with VERT, *Operations Research*, **29**(4), pp.676-697.
[15] Pristker A.A.B. and Happ W.W. (1966) GERT: graphical evaluation and review techniques, Part I (Fundamentals), *Journal of Industrial Engineering,* **17**(5), pp.267-274.
[16] Pristker A.A.B., Whitehouse G.E. (1966) GERT: graphical evaluation and review techniques, Part II (Probabilistic and industrial engineering applications), *Journal of Industrial Engineering*, **17**(6), pp.293-301.
[17] Pristker A.A.B. (1977) *Modelling and Analysis Using Q-GERT Networks*. New York: John Wiley.
[18] Voropajev V.I., Lubkin S.M., Tirazenko B.P., Golenko-Ginzburg D. (2000) Structural Classification of Network Models, *International Journal of Project Management*, **18**, pp.361-368.
[19] Whitehouse G.E. (1973) *System Analysis and Design Using Networks Techniques*. New Jersey: Prentice-Hall, Englewood Cliffs.
[20] Xespos R.F. and Strassman P.A. (1965) Stochastic Decisions Trees for the Analysis of Investment Decisions, *Management Science B***, 11**, pp.244-259.

Received on the 21st of May 2005

Computer Modelling and New Technologies, 2005, Vol.9, No.1, 47-56
Transport and Telecommunication Institute, Lomonosov 1, LV-1019, Riga, Latvia

АЛГОРИТМЫ РАСПРЕДЕЛЕНИЯ СТОИМОСТНЫХ РЕСУРСОВ В ПРОЕКТНО-КОНСТРУКТОРСКОМ БЮРО

А.И. КРАВЧЕНКО[*], С.М. ЛЮБКИН*, В.С. РЕЗЕР*, А. БЕН-ЯИР, А.В. МАЛЫШЕВА****

[*] Российская Ассоциация Управления Проектами / СОВНЕТ, Москва
***Университет им. Бен-Гуриона, г. Беер-Шева, Израиль*

При формировании сводного тематического плана конструкторского бюро на определенный плановый период рассматривается задача оптимального распределения выделенного на этот период бюджета между отдельными проектами. В качестве критерия оптимальности учитывается обобщенный показатель, включающий степень приоритета по каждому проекту, вероятность выполнения проекта к прогнозируемому сроку, который определяется в процессе решения задачи, а также величину смещения этого срока относительно директивно заданного. Решение задачи основано на использовании метода динамического программирования.

Ключевые слова: *оптимальное распределение бюджета, конструкторское бюро, динамическое программирование*

1. Введение

Рост технического оснащения современных средств и систем приводит к развитию экономико-математических моделей и методов планирования и управления конструкторскими бюро для различных отраслей. При этом возникает необходимость постановки и последующего решения ряда оптимальных задач, основанных на распределении ресурсов между несколькими проектами.

При формировании сводного тематического плана конструкторского бюро на определенный плановый период T (год, квартал и т. д.) возникает задача оптимального распределения выделенного на этот период суммарного ресурса C_T между отдельными разработками (проектами). В рассматриваемой ниже постановке задачи под суммарным ресурсом, подлежащим распределению, подразумевается суммарный объем всех ресурсов, выраженный в виде единого эквивалента – в стоимостных единицах. Учитывая то обстоятельство, что директивные сроки выполнения каждой из разработок могут (в общем случае) превосходить конец планового периода, необходимо заложить в критерий оптимизации степень реализуемости проектов в заданные сроки. При распределении затрат необходимо также выдерживать ряд ограничений на динамику потребления затрат не только в течение рассматриваемого планового периода T, но также и после планового периода – до момента окончания всех разработок.

Из сказанного следует, что исходная информация для математической постановки задачи распределения затрат между проектами содержит два важнейших элемента:

а) элемент прогнозирования хода разработок по некоторой обобщенной характеристике (например, относительную трудоемкость) при определении варианта распределения затрат между проектами;

б) элемент формирования критерия как числовой функции, зависящей от показателей прогноза (например, вероятность выполнения или невыполнения плана), а также ограничений задачи.

Элемент прогнозирования должен содержать максимально возможную информацию о ходе выполнения разработок после рассматриваемого периода T. Выполняемые разработки в момент планирования могут находиться в различных состояниях: на стадии аванпроекта, эскизного проекта, опытного производства, испытаний, серийного производства. Поэтому уровень неопределенности при прогнозировании для каждой стадии различен и, естественно, убывает при последовательном переходе на очередную стадию. Модели, отражающие отдельные объекты новой техники, могут быть представлены сетевыми графиками детерминированного и стохастического типов, как по топологии, так и по оценкам выполнения каждой из работ.

Задача оптимального распределения затрат между проектами, представленными сетевыми графиками, в общем случае является экстремальной задачей большой размерности. Опыт решения подобных задач для сетевых моделей различного объема (см., например, [1]) показал, что их реализация связана со значительными вычислительными трудностями, если речь идет о точном решении, или возможно лишь приближенное решение. Учитывая то обстоятельство, что сетевые модели, отражающие ход выполнения разработок, в процессе оперативного управления подвергаются изменениям, как по топологии, так и по продолжительности оценок выполнения отдельных работ, а также, принимая во внимание сложность решения многоразмерных экстремальных задач на сетях, можно считать рассмотренную постановку излишне громоздкой.

В задаче оптимального распределения затрат между разработками, рассматриваемой в данном исследовании, сетевые модели используются лишь на этапе прогнозирования сроков выполнения разработок при условии, если задано распределение затрат между ними. В этом случае, если отдельные стадии выполнения разработок недостаточно адекватно описываются сетевыми моделями (например, стадия аванпроекта), динамика хода выполнения таких разработок описывается случайными процессами простейшего типа с заданными функциями математических ожиданий и дисперсий. Способы построения характеристик этих процессов рассмотрены нами ниже.

2. Постановка математических задач

Для математического описания поставленной задачи предварительно введем следующие обозначения:

N - количество рассматриваемых разработок;

$\Pi = [\pi_1,...,\pi_N]$ - заданные приоритеты разработок;

$C = [C_1,...,C_N]$ - полные стоимости разработок;

$\vec{t}_\Phi = [t_1,...,t_N]$ - время, истекшее с начала выполнения разработок;

$S_{дир} = [S_1,...,S_N]$ - директивные сроки окончания разработок;

$P = [P_1,...,P_N]$ - заданные вероятности выполнения разработок;

$D = [d_1,...,d_N]$ - ограничения на максимальную скорость потребления ресурса;

$Q = [q_1,...,q_N]$ - относительная трудоемкость выполнения работ по каждой разработке на начало планируемого периода; $0 \le q \le 1$, $i = \overline{1,N}$;

T - величина периода планирования (год, месяц);

C_T - размер ресурса, подлежащего распределению;

C^0 - директивное распределение суммарного ресурса во времени;

$\vec{x} = [x_1,...,x_N]$ - искомый вектор, определяющий приращение относительной трудоемкости на плановый период T по каждой разработке;

$\vec{\tau} = [\tau_1,...,\tau_N]$ - времена окончания выполнения каждой разработки, которые определяются в результате решения задачи;

t^0 - рассматриваемый момент планирования;

$\xi_k(t)$ - заданный случайный процесс, определяющий распределение относительной трудоемкости выполнения k-й разработки в момент времени $t > t^0 + T$.

Предполагается, что

$$\xi_k(t) = m_k(t) + \varepsilon_k(t), \qquad (1)$$

где $m_k(t)$ - заданная детерминированная монотонно неубывающая функция; $\varepsilon_k(t)$ - некоррелированный случайный процесс с нулевой функцией математического ожидания; $\sigma_k(t)$ - среднеквадратическое отклонение случайной величины $\varepsilon_k(t)$ в момент времени t.

Предполагается также, что функция $\sigma_k(t)$ является неубывающей.

В данной работе при оценке параметров рассмотренного случайного процесса (1) будем ограничиваться лишь первыми его двумя моментами.

Задавая по каждой k-й разработке величины x_k и τ_k, можно вычислить вероятность ее выполнения по формуле:

$$F_k(x_k,\tau_k)=P\{q_k+x_k+\xi_k(\tau_k-t^0-T)\geq 1\}. \quad (2)$$

Формула (2) позволяет вычислить вероятность того, что случайный процесс, имеющий в качестве начального состояния точку Γ с координатами (t^0+T, q_k+x_k) (рис. 1), в момент времени τ_k выйдет из полосы единичной ширины.

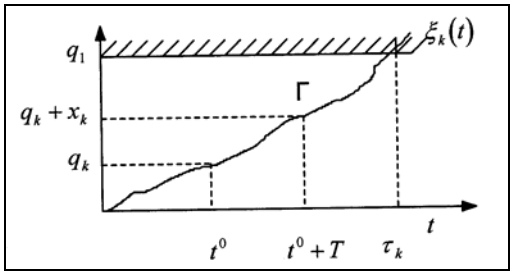


Рис. 1. Оценка параметров случайного процесса

Критерий оптимальности распределения затрат между проектами должен учитывать в прямой зависимости приоритетность π_k каждой разработки, вероятность ее выполнения к моменту окончания τ_k и величину смещения этого срока относительно директивно заданного. В данной постановке задачи предлагается формула для критерия W:

$$W(\vec{x},\vec{\tau})=\sum_{k=1}^{N}\pi_k[1-F_k(x_k,\tau_k)](\tau_k-S_k)^2, \quad (3)$$

где $F_k(x_k,\tau_k)$ вычисляется по формуле (2).

Переходим теперь к математической постановке исходной задачи.

Пусть область D всех допустимых векторов $\vec{x}$ и $\vec{\tau}$, характеризующих всевозможные варианты распределения затрат между проектами, определяется следующими неравенствами:

$$F_k(x_k,\tau_k)-P_k\geq 0; \quad (4)$$

$$\sum_{k=1}^{N}x_kC_k-C_T\leq 0; \quad (5)$$

$$x_k\leq\min(1-q_k,d_k); \quad (6)$$

$$\Phi(t)=\widetilde{P}-P\left\{\sum_{k=1}^{N}C_k\cdot[q_k+x_k+\xi_k(t)]\leq C^0(t^0+T+t)\right\}\leq 0, \quad (7)$$

где $0\leq t\leq\tau_k-(t^0+T)$.

В формулах (4-7) предполагается, что $k=\overline{1,N}$. Неравенство (4) отражает то требование, чтобы вероятность выполнения каждой разработки превосходила заданный уровень P_k. Неравенство (5) требует, чтобы планируемые приросты относительных трудоемкостей по каждой разработке соответствовали суммарным затратам, не превосходящим заданного значения C_T.

Кроме того, приросты относительных трудоемкостей по каждой разработке не должны превосходить заданной скорости d_k или же оставшейся относительной трудоемкости. Этот факт отражен в неравенстве (6). Ограничение по динамике потребления ресурса в момент времени $t>t^0+T$ отражено в неравенстве (7).

Требуется найти в области D наилучшую пару векторов $(\vec{x}^*,\vec{\tau}^*)\in D$, которая обращает в минимум функцию вида (3). Другими словами, должно выполняться соотношение:

$$W(\vec{x}^*,\vec{\tau}^*)=\min_{(x,\tau)\in D}W(\vec{x},\vec{\tau}). \quad (8)$$

Прежде чем переходить к описанию алгоритмов решения задачи (4-8), остановимся подробнее на свойствах функции $F(x,\tau)$, вид которой представлен в (2). При конструировании алгоритмов

нас будут интересовать условия, налагаемые на случайный процесс $\xi(t)$, при выполнении которых функция $F(x,\tau)$ является для любого x неубывающей функцией τ.

При любом $\tau > 0$ выражение для $F(x,\tau)$ имеет вид:

$$F(x,\tau) = \frac{1}{\sigma(\tau)\sqrt{2\pi}} \int_1^{\infty} \exp\left[-\frac{(z - E(\tau))^2}{2\sigma^2(\tau)} \right] dz,$$

где E – символ математического ожидания.

Используя преобразование $\varphi(z,\tau) = \frac{z - E(\tau)}{\sigma(\tau)}$, перепишем выражение для $F(x,\tau)$ в следующем виде:

$$F'(x,\tau) = \frac{1}{\sqrt{2\pi}} \int_{\varphi(1,\tau)}^{\infty} \exp\left[-\frac{\varphi^2}{2} \right] d\varphi.$$

Формула для вычисления производной интеграла, зависящего от параметра τ, приводит к выражению для

Так как $\varphi'_\tau(1,\tau) = \frac{-E'\sigma - (1-E)\sigma'}{\sigma^2}$, то условие, накладываемое на параметры случайного процесса $\varepsilon(t)$, которое приводит к монотонному неубыванию по t функции $F(x,\tau)$, состоит в следующем:

$$E'(\tau)\sigma(\tau) > [E(\tau) - 1]\sigma'(\tau). \qquad (9)$$

Очевидно, условию (9) удовлетворяют широко используемые на практике случайные процессы с линейными функциями $E(\tau)$, $\sigma(\tau)$.

При выполнении условия (9) каждое слагаемое функции $W(x,\tau)$ в формуле (3) при заданном x_k достигает минимального (нулевого) значения при $\tau_k = S_k - (t^0 + T)$. Если же на τ_k накладывается ограничение (4), то каждое слагаемое $W(\vec{x},\vec{\tau})$ достигает минимального значения при

$$\tau_k = \max[S_k - t^0 - T,\ b], \qquad (10)$$

где b удовлетворяет соотношению:

$$\Phi\left[\frac{1 - E(t^0 + T + b)}{\sigma(t^0 + T + b)} \right] = P_k + \frac{1}{2}, \qquad (11)$$

где $\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_0^x e^{-\frac{y^2}{2}} dy$ - функция Лапласа.

Разработанные и описанные ниже алгоритмы позволяют найти решение поставленной выше задачи (4-8) в два этапа: а) этап решения задачи № 1 (4-8) без учета ограничения (7) и б) этап перехода к решению исходной задачи с учетом ограничения (7) – задача № 2.

3. Численная реализация поставленных задач

Численная реализация задачи № 1 основана на базе использования метода динамического программирования. Численная реализация задачи № 2 и оптимального распределения в целом приводится в комплексном алгоритме, который описан в конце данной работы в операторном виде. Прогнозирование динамики изменения оставшейся трудоемкости осуществляется на базе использования регрессионной модели процесса разработки (как правило, линейной). При определении характеристик случайного процесса $\xi_k(t)$, отражающего распределение относительной трудоемкости выполнения k-й разработки в момент времени $t > t^0 + T$, будем считать, что трудоемкость на отрезке $[t^0 + T, \tilde{\tau}_k]$ нарастает постоянно.

Другими словами, уравнение для функции математического ожидания случайного процесса, отражающего ход выполнения разработки при $t > t^0 + T$, имеет вид:

$$m_k(t) = At + B. \quad (12)$$

Коэффициенты A и B выбираются так, чтобы искомая прямая проходила через две точки, одна из которых имеет координаты $\left(t^0 + T, q_k + x_k\right)$, а другая - $\left(S_k, Q_k\right)$. Координата Q_k подлежит определению, исходя из условия:

$$\frac{1}{\sigma_k\sqrt{2\pi}} \int_{-\infty}^{1} \exp\left[-\frac{(x-Q_k)^2}{2\sigma_k^2}\right] dx = P_k. \quad (13)$$

Неравенство (13) отражает требование выполнения разработки к директивно заданному сроку S_k с надежностью P_k. Исходя из сказанного, формула для расчета A имеет вид:

$$A = \frac{Q_k - (q_k + x_k)}{\tau_k - (t^0 + T)}. \quad (14)$$

В случае, если на интенсивность (по трудоемкости) выполнения разработки накладывается ограничение (меньше α'), то осуществляется проверка выполнения условия

$A - \alpha' \le 0$.

Если условие не выполняется, то коэффициент $A := \alpha'$.

Таким образом, окончательная формула для расчета коэффициентов A и B имеет вид:

$A = \min(A', \alpha'); B = q_k + x_k$.

Уравнение для функции дисперсии рассматриваемого случайного процесса, исходя из выше упомянутых предпосылок, имеет вид:

$$\sigma_k^2(t) = \frac{\sigma_k^2}{\widetilde{\tau}_k - (t^0 + T)}(t - t^0 - T), \quad (15)$$

где σ_k^2 - значение дисперсии, полученное в результате обработки полученной статистики на базе использования регрессионной модели методом пассивного эксперимента.

$\widetilde{\tau}_k = S_k$, если $A = A'$; или

$\widetilde{\tau}_k = \tau_k$, если $A = \alpha'$;

$$\tau'_k = \frac{1}{\sigma_k(\tau_k^*)\sqrt{2\pi}} \int_{-\infty}^{1} exp\left(-\frac{x - m_k(\tau_k^*)}{2\sigma_k(\tau_k^*)}\right) dx = P_k. \quad (16)$$

Приводим перечень используемой в алгоритме символики:

Δt	-	масштаб времени;
T	-	величина планового периода;
t^0	-	момент начала планового периода;
$C^0(t)$	-	ограничение на динамику затрат для моментов времени $t > t^0 + T$;
P	-	уровень надежности выполнения ограничений (7);
Δy	-	величина начального шага;
ε	-	точность решения;
h	-	параметр настройки алгоритма;
M	-	размер выборки для определения статистического градиента;
M_z	-	максимальное число “неудачных” шагов по статистическому градиенту при фиксированном шаге Δy;
R_3	-	счетчик удачных шагов;
$\vec{x}^* = \left[x_1^*, ..., x_N^*\right]$	-	оптимальный вектор приращения относительной трудоемкости;
$\vec{\tau} = \left[\tau_1, ..., \tau_N\right]$	-	время окончания выполнения проектов с заданной вероятностью P_k при распределении $\vec{x}^*$;
$W(\vec{x}^*, \vec{\tau}^*)$	-	минимальное значение критерия.

Процесс решения задачи № 1 можно представить как одномерный динамический процесс распределения ресурса C_T по N шагам, где N - количество разработок. Это становится возможным, если воспользоваться формулой (10) для расчета τ_k. Найденное τ_k соответствует минимальному значению k-го слагаемого для критерия W. Иначе говоря, существует функциональная зависимость вида:

$$\tau_k = \tau_k(x_k). \tag{17}$$

Используя зависимость (17), можно переписать формулу для критерия W следующим образом:

$$W(\vec{x},\vec{\tau}) = \sum_{k=1}^{N} W_k(x_k) = \sum_{k=1}^{N} \pi_k \left[1 - F_k(x_k, \tau_k\{x_k\})\right]\left[t_0 + T + \tau_k(x_k) - S_k\right]^2, \tag{18}$$

где формула (18) представляет собой аддитивную функцию каждой компоненты вектора $\vec{x}$.

Переходим теперь к описанию алгоритма, предварительно введя систему обозначений:

k - номер шага распределения (номер проекта);

$\vec{x}^k = [x_1,...,x_k]$ - вектор, определяющий приращение относительной трудоемкости на плановый период T до k-го шага включительно;

$\vec{y}^k = f(\vec{x}^k) = [y_1,...,y_k]$ - вектор накопленных затрат, отражающий динамику распределения $\vec{x}^k$.

Каждая компонента вектора $\vec{y}^k$ подсчитывается по формуле:

$$y_k = \sum_{j=1}^{k} C_j x_j \ . \tag{19}$$

$W[y_1^*,...,y_k^*]$ - величина целевой функции, соответствующая оптимальному распределению затрат $\vec{x}^*(k)$.

Использование принципа оптимальности [2] приводит к следующему соотношению:

$$W[y_1^*,...,y_k^*] = \min_{\{x_k : x_k + y_{k-1}^* = y_k^*;\, x_k \in D\}} \left\{W[y_1^*,...,y_{k-1}^*] + W_k(x_k)\right\},\ k = 2,...,N, \tag{20}$$

где область D определяется неравенствами (4-6).

3.1. АЛГОРИТМ РЕШЕНИЯ ЗАДАЧИ № 1

В алгоритме осуществлена вычислительная реализация метода динамического программирования [2] с некоторым шагом дискретности Δ. На каждом шаге распределения k вычисляется разброс возможных накопленных затрат $J_k \cdot \Delta$, подлежащих распределению. Для каждого значения затрат $y_k^j = j \cdot \Delta$, где $j = \overline{1, J_k}$, просматривается множество возможных вариантов и запоминается наилучший. Множество возможных вариантов распределения после k шагов, требующих затрат размером y_k^j, определяется в результате продолжения оптимальных вариантов распределения после $(k-1)$-го шага. Эти варианты хранятся в памяти компьютера. Просмотр вариантов распределения осуществляется путем введения составного цикла, состоящего из трех вложенных друг в друга простых циклов: цикла просмотра шагов $k = \overline{1, N}$, цикла просмотра различных уровней затрат на каждом шаге $j = \overline{1, J_k}$ и цикла просмотра всех вариантов, требующих затрат, равных $y_k^j = j \cdot \Delta$, $s = \overline{1, J_{k-1}}$. В результате работы алгоритма на печать выдается множество оптимальных вариантов распределения после N-го шага, каждый из которых требует различных размеров затрат с равным шагом дискретности, а именно $y_N^j = j \cdot \Delta$, где $j = \overline{1, J_N}$, а $J_N = \left[\frac{C_T}{\Delta}\right] + 1$.

Символ $[x]$ определяет целую часть величины x, не превосходящую x.

Переходим к описанию используемых в алгоритме операторов:

Оператор L_1 осуществляет присваивание $k := 1$, где k - номер шага.

Оператор L_2 осуществляет присваивание $y_0' := 0$, где y_0' - величина затрат на нулевом шаге.

Оператор L_3 осуществляет присваивание $W_0 := 0$, где W_0 - величина критерия на нулевом шаге.

Оператор L_4 осуществляет присваивание $J_0 := 1$, где J_0 - количество возможных вариантов на нулевом шаге.

Таким образом, операторы $L_1 - L_4$ осуществляют подготовку данных для работы алгоритма.

Оператор L_5 осуществляет присваивание $j := 1$, где j - индекс, определяющий уровень затрат на k-м шаге, а именно $y = j \cdot \Delta$.

Оператор A_6 вычисляет уровень накопленных затрат на k-м шаге, соответствующий индексу j по формуле:

$$y_k^j = j \cdot \Delta .$$

Оператор L_7 присваивает $s := 1$, где s - индекс, соответствующий номеру варианта распределения до k-го шага включительно и приводящего к уровню затрат, равному y_k^j.

Оператор A_8 вычисляет величину приращения относительной трудоемкости x_k^s, приводящей к заданному уровню по формуле:

$$x_k^s = \frac{y_k^j - y_{k-1}^s}{C_k} .$$

Оператор P_9 осуществляет проверку выполнения условия $x_k^s \geq 0$. Если условие не выполняется, то происходит передача управления оператору L_{14}.

Оператор P_{10} осуществляет проверку выполнения условия $x_k^s \in D$, где D - область, определяемая неравенствами (4-6). Если условие не выполняется, то происходит передача управления оператору L_{14}.

Оператор A_{11} вычисляет величину критерия B_k, соответствующего s-му наилучшему варианту до $(k-1)$-го шага с величиной приращения x_k^s на k-м шаге. Величина критерия подсчитывается по формуле:

$$B_k^s = W_{k-1}^s + W_k^j\left(x_k^s\right). \qquad (21)$$

В формуле (21) W_{k-1}^s - величина критерия, соответствующая наилучшему варианту распределения до $(k-1)$-го шага с уровнем затрат, равным y_{k-1}^s; $W_k^j\left(x_k^s\right)$ - слагаемые суммы в формуле (3).

Оператор P_{12} проверяет выполнение условия $B_k^s - W_k^j \geq 0$. Если условие выполняется, то s-й вариант не является наилучшим и происходит передача управления оператору L_{14}.

Оператор 3_{13} работает в условиях, когда s-й вариант является наилучшим и осуществляет запоминание $W_k^j = B_k^s$ и уровня y_{k-1}^s.

Оператор L_{14} осуществляет переход к просмотру очередного варианта путем присваивания очередного номера счетчика $s := s + 1$.

Оператор P_{15} проверяет выполнение условия $s > y_{k-1}$. Если условие не выполняется, то это означает, что просмотрены не все варианты. Осуществляется переход к просмотру очередного варианта на оператор A_8.

Оператор L_{16} осуществляет переход к просмотру вариантов, приводящих к уровню затрат y_k^{j+1}, т.е. присваивание $j := j + 1$.

Оператор P_{17} проверяет выполнение условия $j > y_k$. Если условие не выполняется, то происходит передача управления на начало просмотра вариантов, т.е. к оператору A_6.

Оператор L_{18} работает в условиях, когда на k-м шаге все операции выполнены и осуществляется начало работы на $(k+1)$-м шаге, т.е. осуществляется присваивание $k := k+1$.

Оператор P_{19} проверяет выполнение условия $k > N$. Если условие не выполняется, то происходит передача управления на окончание процедуры, т.е. к оператору $Я_{24}$.

Оператор A_{20} вычисляет границы изменения затрат на k-м шаге по формуле:

$$J_k = J_{k-1} + \frac{C_k \cdot \min\left[1 - \frac{J_{k-1}}{C_k},\ d_k\right]}{\Delta}.$$

Оператор Q_{21} передает управление оператору L_5.

Оператор 3_{22} запоминает пары $\left(W_k^j, y_k^j\right)$, $\left(W_{k-1}^{s(j)}, y_{k-1}^{s(j)}\right)$ для любых j.

Оператор A_{23} вычисляет $W_N^{j^*} = \min\limits_j W_N^j$.

Оператор $Я_{24}$ реализует окончание алгоритма, производит печать необходимой выходной информации по оптимальному варианту распределения:

$\vec{y}^* = \left[y_1^*, ..., y_N^*\right], x = \left[x_1, ..., x_N\right], W(\vec{x})$, где $x_i = \frac{y_i - y_{i-1}}{C_i}$, $i = \overline{1, N}$, $x_0 = 0$.

Операторная схема алгоритма при описанных выше операторах имеет вид:

$L_1 L_2 L_3 L_4 L_5 A_6 L_7 A_8 P_{9\downarrow 14} P_{10\downarrow 14} A_{11} P_{12\uparrow 14} 3_{13} L_{14} P_{15\downarrow 8} L_{16} P_{17\downarrow 6} L_{18} P_{19\downarrow 24} A_{20} Q_{21} 3_{22} A_{23} Я_{24}$.

Переходим к алгоритму решения исходной задачи (задачи № 2). Ввиду того, что для требуемого суммарного ресурса C_T, соответствующего решению задачи (4-6, 8) условие (7) при некоторых t может не выполняться, требуется осуществить оптимальное “сжатие” или “растяжение” времени выполнения проектов в зависимости от превышения или недостатка наличного ресурса $C^0(t)$ над требуемым C_T.

Будем полагать, что изменение величины приращения x_k относительной трудоемкости на некоторую величину Δx_k вызывает изменение времени выполнения на некоторую величину $\Delta\tau_k$:

$$\Delta\tau_k = \varphi(\Delta x_k).$$

Задача оптимального “растяжения” времени выполнения каждого проекта сводится к отысканию такого вектора

$$\Delta\vec{x} = \left[\Delta x_1, ..., \Delta x_N\right]$$

в любой момент времени t, при котором выполняется ограничение

$$P\left[C_t(\vec{x} + \Delta\vec{x}(t)) \le C^0(t)\right] \ge P \qquad (22)$$

и критерий

$$W(\Delta x(t)) = \sum_{N(t)} \pi_k (1 - P_k)\left[t_k^0 + T + t + \Delta t_k - S_k\right]^2 \qquad (23)$$

достигает минимального значения.

В формуле (23) $N(t)$ представляет собой множество разработок, выполнение которых не окончено к рассматриваемому моменту времени t.

Переходим к описанию алгоритма решения задачи № 2. Прилагаемый ниже алгоритм основан на методе получения статистического градиента функционала $W(\vec{x}, \vec{\tau})$ с проектированием его на границу допустимой области, определяемой ограничениями (4-7).

3.2. АЛГОРИТМ РЕШЕНИЯ ЗАДАЧИ № 2

Алгоритм реализует поиск локального экстремума $\vec{x}^* = \left[x_1^*,...,x_N^*\right]$, отражающего оптимальное распределение ресурсов между разработками. К основным блокам рассматриваемого алгоритма можно отнести следующее: формирование исходного допустимого вектора $\vec{x}^0$, удовлетворяющего ограничениям (4-7); вычисление стохастического градиента $grad\,W\left(\vec{x}^k\right)$ в рассматриваемой точке $\vec{x}^k$; проектирование вектора $grad\,W\left(\vec{x}^k\right)$ на поверхность ограничений (4-7); вычисление вектора $\vec{h}\left(\vec{x}^k\right)$; вычисление шага продвижения вдоль вектора $\vec{h}\left(\vec{x}^k\right)$; реализация окончания процедуры.

3.3. ОПЕРАТОРНАЯ СХЕМА

Q_1 - ввод исходной информации.

A_2 - вычисление вектора $\vec{x}^0$ в результате решения задачи № 1.

A_3 - вычисление моментов окончания разработок $\tau = \tau\left(\vec{x}^0\right)$ на основе (10).

A_4 - вычисление левых частей неравенства (7). $\Phi\left(t,\vec{x}^0\right)$ при $t = \Delta t,\ 2\Delta t,...,\ n\Delta t$.

P_5 - проверка условия $\Phi\left(t,\overline{x^0}\right) \le 0$ при всех t. Если да, то переход к $Я_{19}$.

A_6 - выделение j^*: $\Phi\left(t_{j^*},x^0\right) = \min\Phi\left(t_j,...,x^0\right)$.

A_7 - вычисление $grad\,\Phi\left(t_{j^*},x^0,\tau^0\right) = \left[\dfrac{\partial\Phi}{\partial x^0},\dfrac{\partial\Phi}{\partial\tau^0}\right]$.

A_8 - вычисление $h\left(x_0\right)$ - проекции $grad\,\Phi\left(t_{j^*},x^0\right)$ на плоскость (5).

A_9 - определение $x^0 := x^0 - \alpha_1\dfrac{\partial\Phi}{\partial x^0} - \alpha_2\dfrac{\partial\Phi}{\partial\tau^0}$, где $\alpha_1,\ \alpha_2 > 0$.

A_{10} - вычисление $\Phi\left(t_{j^*},x^0,\tau^0\right)$.

P_{11} - проверка условия $\Phi\left(t_{j^*},x^0\right) \le 0$. Если нет, то переход к A_6.

A_{12} - $k := 0$.

A_{13} - вычисление $W\left(\vec{x}^k,\vec{\tau}^k\right)$.

A_{14} - вычисление $W\left(\vec{x}^k,\vec{\tau}^k\right) = \left[\dfrac{\partial W}{\partial\overline{x^k}},\dfrac{\partial W}{\partial\overline{\tau^k}}\right]$.

A_{15} - вычисление $h\left(\vec{x}^k,\vec{\tau}^k\right)$ - проекции $grad\,W\left(\vec{x}^k,\vec{\tau}^k\right)$ на плоскость, касательную к (7).

P_{16} - проверка $\dfrac{\left\|h\left(\vec{x}^k,\vec{\tau}^k\right)\right\|}{\left\|grad\,W\left(\vec{x}^k,\vec{\tau}^k\right)\right\|} < \delta$. Если да, то переход к $Я_{19}$.

A_{17} - $k := k + 1$.

F_{18} - переход к A_{13}.

$Я_{19}$ - окончание работы алгоритма.

Операторная схема алгоритма имеет следующий вид:

$$Q_1A_2A_3A_4P_{5\uparrow19}A_6A_7A_8A_9A_{10}P_{11\downarrow6}A_{12}A_{13}A_{14}A_{15}P_{16\uparrow19}A_{17}F_{18}Я_{19}.$$

4. Выводы

- Рассмотрена и решена оптимальная задача распределения выделенного конструкторскому бюро (КБ) бюджета между разработками (проектами) КБ. В качестве критерия оптимальности учитывается обобщенный показатель, включающий степень приоритета по каждому проекту, вероятность выполнения проекта к прогнозируемому сроку, который определяется в процессе решения задачи, а также величину смещения этого срока относительно директивно заданного.
- Решение задачи осуществляется в два этапа. Численная реализация первого этапа основана на использовании метода динамического программирования. На последующем этапе реализуется комплексный алгоритм, который использует ограничение по динамике потребления ресурса. Оптимизация распределения ресурсов между разработками осуществляется на основе поиска локального экстремума.

Литература

[1] Голенко Д., Лившиц С., Кеслер С. (1977) *Статистическое моделирование в технико-экономических системах (Управление разработками).* Ленинград: Изд. Ленинградского Университета. 264 с.

[2] Taha H.A. (1997) *Operations Research. An Introduction.* New York: Collier Macmillan. 916 p.

Received on the 21st of May 2005

Computer Modelling and New Technologies, 2005, Vol.9, No.1, 57-67
Transport and Telecommunication Institute, Lomonosov 1, LV-1019, Riga, Latvia

DECISION SUPPORT WEB-BASED SYSTEM FOR CONSTRUCTION INNOVATION

E.K. ZAVADSKAS, A. KAKLAUSKAS, M. VITEIKIENE

Vilnius Gediminas Technical University,
Sauletekio al. 11, 10223 Vilnius, Lithuania.
Ph. (+3705) 2745002, Fax. (+3705) 2700114. E-mail: edmundas.zavadskas@adm.vtu.lt

Many construction and facilities management Web sites can be found on the Internet. The interested parties on construction and facilities management Web sites can find databases of best practices, analysers, software, expert and decision, etc.

Technological innovation mainly through changes in the availability of information and communication technology inclusive databases of best practices, calculators, analysers, software, neural networks, decision support and expert systems that have been provided by a variety of new services developed by the construction and facilities management sectors.

Most of all calculators, analysers, software, decision support and expert systems, neural networks and on-line systems seek to find out how to make the most economic decisions and most of all these decisions are intended only for economic objectives. Alternatives under evaluation have to be evaluated not only from the economic position, but take into consideration qualitative, technical, technological and other characteristics as well. Based on the analysis of the existing calculators, analysers, information, expert and decision support systems, neural networks and in order to determine most efficient versions of best practices a Decision Support Web-Based System for Construction Innovation (*IDSS*) was developed by Vilnius Gediminas Technical University.

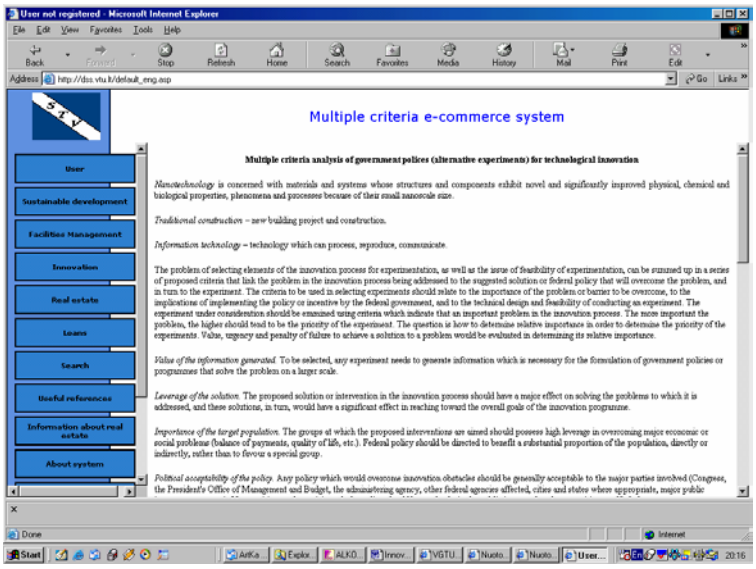
Innovation activities involve a number of interested parties who pursue various goals and have different potentialities, educational levels and experiences. This leads to various approaches of the above parties to decision-making in this field. In order to do a full analysis of the available alternatives and to obtain an efficient compromise solution, it is often necessary to analyze economic, technical, technological, management, organization, legal, social and other information. This information should be provided in a user-oriented way.

Keywords: construction, innovation, decision support system, multiple criteria

1. WEB-Based innovation decision support system

Based on the analysis of the existing calculators, analyzers, information, expert and decision support systems, neural networks and in order to determine most efficient versions of best practices a Web-Based Innovation Decision Support System (*IDSS*) was developed by VGTU. *IDSS* consisting of a database of best practices, database management system, model-base, model-base management system and user interface.

1.1. DATABASE OF BEST PRACTICE



Innovation activities involve a number of interested parties who pursue various goals and have different potentialities, educational levels and experiences. This leads to various approaches of the above parties to decision-making in this field. In order to do a full analysis of the available alternatives and to obtain an efficient compromise solution, it is often necessary to analyze economic, technical, technological, management, organization, legal, social and other information. This

information should be provided in a user-oriented way. The presentation of information needed for decision-making in the *IDSS* may be in a conceptual form (i.e. digital/numerical, textual, graphical, diagrams, graphs and drawing, etc), photographic, sound, video and quantitative forms. The presentation of information needed for decision-making in the IDSS may be in a textual form.

The presentation of quantitative information involves criteria systems and subsystems, units of measurement, values and initial weights that fully define the provided variants. Conceptual information means a conceptual description of the alternative solutions, the criteria and ways of determining their values and the weights, etc.

In this way, the *IDSS* enables the decision-maker to receive various conceptual and quantitative information's on innovation alternatives from a database of best practice and to make a model-base allowing him/her to analyze the above factors and to form an efficient solution.

The following parts form the *IDSS*'s database of best practice:

- Innovation,
- Construction,
- Facilities Management,
- Real Estate,
- Refurbishment,
- Sustainable Development,
- Loans,
- International Trade,
- Ethics.

The following tables form the *IDSS*'s database:

- Initial data tables. These contain information about the innovations (i.e. real estate, construction, finance, etc.).
- Tables assessing innovation alternatives. These contain quantitative and conceptual information about alternative innovation solutions: finance, information and Internet technologies, facilities management, real estate management, etc.

The user seeking for an efficient innovation solution should provide, in the tables assessing innovation solutions, the exact information about alternatives under consideration as to the client's financial situation. It should be noted that various users making a multiple criteria analysis of the same alternatives often get diverse results. This may be due to the diversity of the overall aims and financial positions of the users. Therefore, the initial data provided by various users for calculating the innovation project differ and consequently lead to various final results.

The character of the objective's choice for the most efficient variant is largely dependent on all available information. It should also be noted that the quantitative information is objective. The actual innovation alternatives have real costs. The values of the qualitative criteria are usually rather subjective though the application of an expert's methods contributes to their objectivity.

The tables assessing innovation solutions are used as a basis for working out the matrices of decision-making. These matrices, along with the use of a model-base and models, make it possible to perform a multiple criteria analysis of alternative innovation projects, resulting in the selection of the most beneficial variants.

1.2. MODEL-BASE

The efficiency of an innovation variant is often determined by taking into account the economic, technical, technological, management, organization, legal, social and other factors. These factors include an account of the economic, aesthetic, technical, technological, management, space, comfort, legal, social and other factors. The model-base of a decision support system should include models that enable a decision-maker to do a comprehensive analysis of the available variants and to make a proper choice. The following models of a model-base aim at performing the functions of:

- A model for the establishment of the criteria weights,
- A model for multiple criteria analysis and for setting the priorities,
- A model for the determination of a project's utility degree,
- A model for the determination of a project's market value.

According to the user's needs, various models may be provided by a model management system. When a certain model (i.e. search for innovation alternatives) is used the results obtained become the initial data for some other models (i.e. a model for multiple criteria analysis and setting the priorities).

The results of the latter, in turn, may be taken as the initial data for some other models (i.e. determination of utility degree of alternatives).

The management system of the model base allows a person to modify the available models, eliminate those that are no longer needed and add some new models that are linked to the existing ones.

Since the analysis of innovations usually performed by taking into account the economic, technical, technological, management, organisation, legal, social and other factors, a model-base should include models which will enable a decision-maker to carry out a comprehensive analysis of the available variants and make a proper choice. The following multiple criteria analysis methods and models as developed by the authors (Kaklauskas, 2002, Zavadskas, 2002) are used by the *IDSS* in the analysis of the innovation alternatives:

1. A new method and model of complex determination of the weight of the criteria taking into account their quantitative and qualitative characteristics was developed. This method allows one to calculate and co-ordinate the weights of the quantitative and qualitative criteria according to the above characteristics.
2. A new method and model of multiple criteria complex proportional evaluation of projects enabling the user to obtain a reduced criterion determining the complex (overall) efficiency of the project was suggested. This generalized criterion is directly proportional to the relative effect of the values and weights of the considered criteria, on the efficiency of the project.
3. In order to find what price will make a valuated project competitive on the market a method and model for determining the utility degree and market value of projects based on the complex analysis of all their benefits and drawbacks was suggested. According to this method the project's utility degree and the market value of a project being estimated are directly proportional to the system of the criteria and adequately describe them, the values and weights of these criteria.
4. A new method and model of multiple criteria multi-variant design of a project's life cycle enabling the user to make computer-aided design of up to 100,000 alternative project versions was developed. Any project's life cycle variant obtained in this way is based on quantitative and conceptual information.

Application of Multiple Criteria Decision Support Web-Based System for Innovation (*IDSS*) allows one to determine the strengths and weaknesses of each phase and its constituent parts. Calculations were made to find out by what degree one version is better than another and the reasons disclosed why it is exactly so. Landmarks are set for an increase in the efficiency of innovation versions. All this was done argumentatively, basing oneself on criteria under investigation and on their values and weights. This saved users' time considerably by allowing them to increase both the efficiency and quality of innovation analysis.

1.3. TECHNOLOGICAL INNOVATIONS ON WEBSITES

Searching for information about the innovations in construction technologies in the Internet, you may find sites with the data on various analyzers, hardware, and decision-making systems.

These sites provide data on various types of analyzers to be used in considering various situations as well as on innovative construction technologies, including the following issues:

1) PATH. The development of residential housing based on public or private initiative to achieve wider application of technologies aimed to improve dwelling quality, durability, energy efficiency and the environment in the USA.

PATH means cooperation with the leading housing managers, product development, insurance and financial activities including state investments in this housing programme. PATH partners ensure quality both for new and existing dwellings, the construction technologies and support new ideas.

PATH also accelerates the implementation of new housing technologies: providing more recent information about construction technologies and systems; resenting new projects to be beneficially used by builders and dwelling owners; developing networks of the authorities, universities and industrial enterprises; eliminating the barriers for transferring the innovations and using the effective methods of product realization.

This is an information system providing the information about new materials, technologies, projects and an opportunity to communicate with experts.

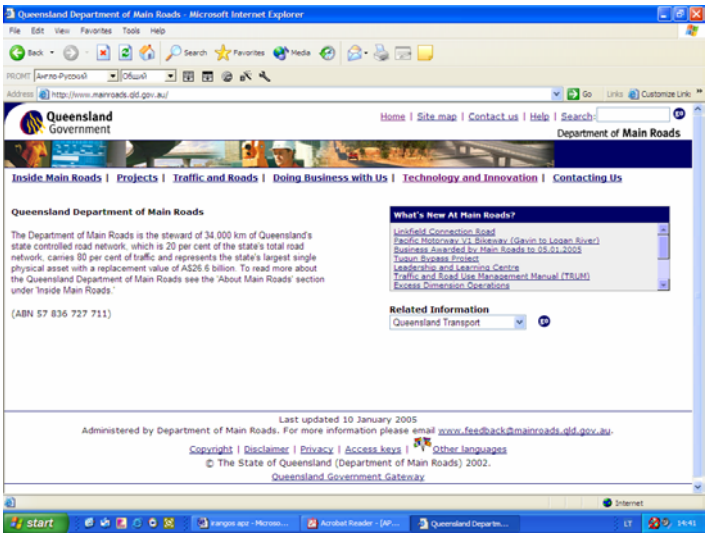
The network of manufacturers, industrial enterprises and builders is developed for discussing new ideas and prospects and presenting them to users as the innovations in housing construction. New advanced construction methods are also debated with governmental institutions and the funding is obtained if necessary.

PATH regularly communicates with the partners, coordinating, planning and controlling its activities.

2) Australian centre for innovation in construction. This centre develops new technologies as well as

providing new tools and management systems to improve the effectiveness of construction. It has more than 150 researchers and partners supporting its activities associated with construction innovation.

The research center for innovation in construction is widely used and developed. Its main goal is to create tools, technologies and management systems to develop the innovative construction industry for the financial, social and environmental benefits to the community. The center of cooperative research is focused on the construction and management.



3) The institute of technological innovation has a large design knowledge database.

4) MOCA. Innovations in Construction: from A to Z. This is implemented by using new technologies (electronic devices, special programs, the Internet).

5) ERIK. ERIK is a network of innovative actions in the European region focused on the theme "Regional Economics Based on Knowledge and Technological Innovation".

ERIK's main aim is to develop networking of regional organizations to provide information to various regions trying to attract the attention of ERDF to the development and implementation of innovative programs.

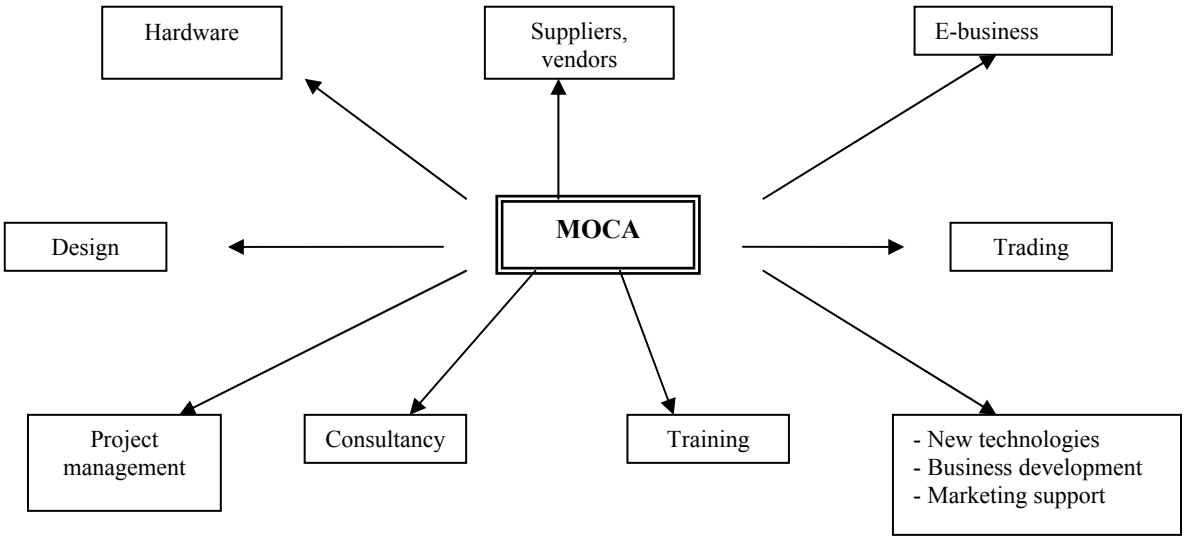
ERIK organizes workshops, study visits, conferences, debate on regional policy, etc. It also runs the website and publishes newsletters. The information is constantly updated.

ERIK is co-funded by the European Commission's DG Regional Policy. 13 partner regions originally funded it. Toscana and Regione Emilia Romagna are coordinators of the network.

ERIK is an open network. Any European region may participate in its activities and the debate on innovation and regional policies. You may contact ERIK with any questions regarding participation in its activities. Programs providing information about the innovation in construction:

1) Egip A6. Software Egip A6 designed for construction area provides information on products, design, and construction in other countries, traditions and different building materials.

2) BIC. BIC is a tool to disseminate information about the innovations in business development. BIC was founded in 1989. It provides data on innovative knowledge in business and the development of small and medium sized companies.



BIC's aim is to help develop innovative SMS, restructure the existing companies and to plan the development of industrial enterprises. BIC plays an important role in providing information and professional advice to less developed regions as well as reducing business risks of the companies. BIC got successful external evaluation and the European Commission's Structural Funds Guidelines for 2000-06 recommended its more intensive use in the implementation of regional programmes.

1.4. DESCRIPTION OF THE EXPERIMENT

Innovations are perceived as natural infiltration of new ideas into the economy resulting in better products, new jobs and manufacture of new items. These ideas and inventions make the necessary condition for innovations to occur.

The government controls the environment where innovations prevail; for example, state employees, a patent system, etc. are the participants of an innovative process, with only few exceptions.

An innovative process includes management organization and human resources. Management is very important making the basis of technological innovations: training of managers and management capabilities are key elements of any company.

Technological changes make an essential feature of modern society. Most people, personally or collectively, contribute to various social changes in such areas as employment, quality of life and economic stability. A continuous development (a mature industry) and economics are likely to rely on investments and resources as well as on the use of technology. Technology is an integral part of mechanization of manufacture. It is mainly centred on labour, products and services satisfying social needs. Various technologies may become the key factor for achieving a higher standard of living.

The goal of the present experiment is both abstract and practical. First, the results obtained due to the application of new technologies, which seem to be most suitable today should be demonstrated. These data may be sufficient for politicians to make the appropriate decisions, implying that the provision of information in due time is very important.

The experiment considered is analysed as an important problem because the importance of the experiment depends on the significance of the problem. Then, the question arises how to determine the problem importance reflecting the relevance of the experiment. Value, haste and sanctions for not implementing the decisions made should be the key factors for the experiment. A comparative analysis of three alternatives based on traditional construction, the use of information technologies in construction and nanotechnology in construction is made.

Applying expert methods processes the data obtained. The values of the criteria are calculated.

The weights of the criteria found by expert methods help to determine how much one particular criterion is more important than another. In the process of criteria evaluation their values are normalized and multiplied by their weights. Therefore, the criteria weights should be harmonized as far as their quantitative and qualitative characteristics are concerned. The weights of all quantitative and qualitative criteria are harmonized. The criteria weights are calculated based on the work [N.Kvederytė, E.K.Zavadskas, A.Kaklauskas 2000].

Using the conceptual approach to the alternatives in question a decision-making matrix is generated. An aggregate weight of the alternatives considered from various perspectives is determined. The weights and priorities of the alternatives are usually determined in five steps: an estimated normalized decision-making matrix D is constructed, the total values of the minimizing S_{-j} and maximizing S_{+j} normalized criteria describing the *j*-th alternative are calculated, the relative weight Q_j of the alternatives is determined and their utility N_j is defined. A detailed description of these stages can be found in the literature [E.K.Zavadskas 1987, E.K.Zavadskas, A.Kaklauskas, L.Simanauskas 1998; N.Kvederytė, E.K.Zavadskas, A.Kaklauskas.2000,].

Problem solution diagram:

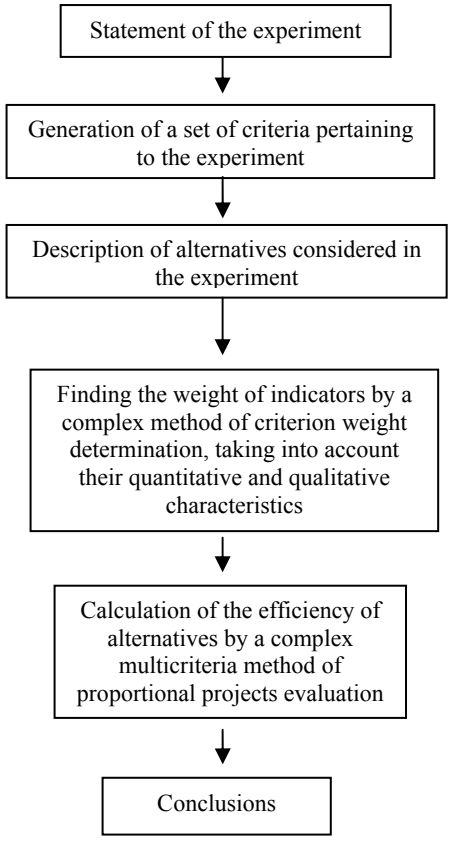


Figure 1. The process of selecting a rational alternative

A decision-making matrix (see Table 1) is generated to determine the efficiency of the considered technological innovations. Then, multicriteria analysis of technological innovations is made. The analysis is based on multicriteria method of proportional evaluation suggested by the authors. The data presented in the tables show that each alternative has some advantages and disadvantages. All the criteria describing the alternatives are scored in points. The higher the scoring, the better is the criterion. The higher the weight of the criterion, the more significant it is for experts and users as well as having greater influence on the final evaluation. Innovations may be considered with the aim to identify the best one capable of winning the market, thereby it may be found which innovation the Government should support.

For this purpose, a decision-making matrix (see Table 1) is generated to consider three alternatives. The criteria for their evaluation were elicited from experts. Then, multicriteria analysis of technological innovations is made. The analysis is based on a multicriteria method of proportional evaluation suggested by the authors [A.Kaklauskas, E.K.Zavadskas 2002].

The data presented in the tables show that each alternative has some advantages and disadvantages. All the criteria describing the alternatives are scored in points. The higher the scoring, the better is the criterion. For example, the data presented in Table 1 show that the criteria values of alternative 2 are higher than those of other options. The higher the weight of the criterion, the more significant it is for experts and users as well as having greater influence on the final evaluation. Let us assume that generating information and the cost of testing get 0.046 and 0.061 points respectively. Then, the latter criterion is by 24.6 % more important than the first one.

TABLE 1. Multiple criteria analysis of government policies for technological innovation (initial calculation data)

Nr.	Criteria under evaluation	Measuring units of criteria	*	Weights of criteria	Information technology in construction	Nanotechnology in construction	Traditional construction
1	Value of the information generated	Points	+	0.046	7,6	9,45	3,333
2	Leverage of the solution	Points	+	0.053	7,6	9,33	6,6
3	Importance of the target population	Points	+	0.052	7,45	9,23	6,6
4	Political acceptability of the policy	Points	+	0.051	5,6	9,66	7
5	Legal aspects of the policy	Points	+	0.044	5,33	4,6	9,33
6	Target population support	Points	+	0.054	6,6	9,33	8
7	Cost acceptability	Points	+	0.054	7	9,33	7,6
8	Policy effectiveness and range	%	+	0.046	6,3	8	6
9	Policy equity	Points	+	0.045	5,6	7,6	6,6
10	Understanding of the policy	Points	+	0.048	5,33	7	9
11	Administrative feasibility	Points	+	0.052	6,3	8	8,6
12	Ease of policy monitoring	Points	+	0.041	5	7,3	5,66
13	Organizational structure for implementation	Points	+	0.055	6,3	8	10
14	Sound experimental hypothesis	Points	+	0.054	7,85	9,33	6,6
15	Careful experimental design	Points	+	0.061	7,6	9,45	9,6
16	Experimental feasibility	Points	+	0.055	7	7,6	9,6
17	Time scale of the experiment	Months	-	0.066	12	9,66	7,3
18	Experimental cost	Points	-	0.061	9,33	10	7,6
19	Relative cost-effectiveness	Points	-	0.054	8	9,33	6,3

The results of calculations based on the application of multicriteria analysis are given in Table 2. The best result is 100%. The data obtained from multicriteria analysis of the alternatives are presented in Table 2.

As shown in the table, Information Technologies are rated by 18.52 % lower than Nanotechnology, while Traditional Construction is rated lower than Nanotechnology by 2.75 %.

The degree of utility of the alternatives compared shows the level of their importance.

According to the data obtained, the Government should support the development of nanotechnology as well as traditional construction because they differ only by 2.75 %. This means that traditional construction is also a very important area. It is hardly possible to state that information technologies are

not important. However, the aim of the present investigation was to identify the area to be supported by the Government. The calculations show that the use of nanotechnology in construction is the most rational option to be supported by the government. However, the economic state of the country is not favourable for making huge investments into a new branch. It is not possible because the financial resources are highly limited.

TABLE 2. Multiple criteria analysis of government policies (alternative experiments) for technological innovation (results)

Criteria under evaluation	Measuring units of criteria	*	Weights of criteria	Weighted normalized values of criteria of the comparable alternatives		
				Information technology in construction	Nanotechnology in construction	Traditional construction
Value of the information generated	Points	+	0.046	0,0172	0,0213	0,0075
Leverage of the solution	Points	+	0.053	0,0171	0,021	0,0149
Importance of the target population	Points	+	0.052	0,0166	0,0206	0,0147
Political acceptability of the policy	Points	+	0.051	0,0128	0,0221	0,016
Legal aspects of the policy	Points	+	0.044	0,0122	0,0105	0,0213
Target population support	Points	+	0.054	0,0149	0,0211	0,0181
Cost acceptability	Points	+	0.054	0,0158	0,0211	0,0172
Policy effectiveness and range	%	+	0.046	0,0143	0,0181	0,0136
Policy equity	Points	+	0.045	0,0127	0,0173	0,015
Understanding of the policy	Points	+	0.048	0,012	0,0158	0,0203
Administrative feasibility	Points	+	0.052	0,0143	0,0182	0,0195
Ease of policy monitoring	Points	+	0.041	0,0114	0,0167	0,0129
Organizational structure for implementation	Points	+	0.055	0,0143	0,0181	0,0226
Sound experimental hypothesis	Points	+	0.054	0,0178	0,0212	0,015
Careful experimental design	Points	+	0.061	0,0174	0,0216	0,022
Experimental feasibility	Points	+	0.055	0,0159	0,0173	0,0218
Time scale of the experiment	Months	-	0.066	0,0273	0,022	0,0166
Experimental cost	Points	-	0.061	0,0211	0,0227	0,0172
Relative cost-effectiveness	Points	-	0.054	0,0183	0,0213	0,0144
The sums of weighted normalized maximizing indices of variant S_{+j}				002367	0,302	0,02724
The sums of weighted normalized minimizing indices of variant S_{-j}				0,667	0,066	0,0482
Significance of variant Q_j				0,29	0,3559	0,3461
Usefulness degree N_j				81,48%	100%	97,25%

1.5. COMPARABLE VARIANT DESCRIPTION

There are three alternatives whose are compare one with other. Nanotechnology is concerned with materials and systems whose structures and components exhibit novel and significantly improved physical, chemical and biological properties, phenomena and processes because of their small nanoscale size. In the construction industry, nanotechnology could potentially improve many construction materials, including structural steel, polymers and concretes. Concrete, which contains the complicated, nanoscale

structures of cement and its hydrates, is an excellent candidate for nanotechnology manipulation and control. Traditional construction – it is a new building project and construction. Information technology – it is technology that can process, reproduce, and communicate.

1.6. VALUE'S CRITERIA

The problem of selecting elements of the innovation process for experimentation, as well as the issue of feasibility of experimentation, can be summed up in a series of proposed criteria that link the problem in the innovation process being addressed to the suggested solution or federal policy that will overcome the problem, and in turn to the experiment. The criteria to be used in selecting experiments should relate to the importance of the problem or barrier to be overcome, to the implications of implementing the policy or incentive by the federal government, and to the technical design and feasibility of conducting an experiment. The experiment under consideration should be examined using criteria, which indicate that, an important problem in the innovation process. The more important the problem, the higher should tend to be the priority of the experiment. The question is how to determine relative importance in order to determine the priority of the experiments. Value, urgency and penalty of failure to achieve a solution to a problem would be evaluated in determining its relative importance.

There are criteria definable these three alternatives:

Value of the information generated. To be selected, any experiment needs to generate information which is necessary for the formulation of government policies or programmes that solve the problem on a larger scale.

Leverage of the solution. The proposed solution or intervention in the innovation process should have a major effect on solving the problems to which it is addressed, and these solutions, in turn, would have a significant effect in reaching toward the overall goals of the innovation programme.

Importance of the target population. The groups at which the proposed interventions are aimed should possess high leverage in overcoming major economic or social problems (balance of payments, quality of life, etc.). Federal policy should be directed to benefit a substantial proportion of the population, directly or indirectly, rather than to favour a special group.

Political acceptability of the policy. Any policy that would overcome innovation obstacles should be generally acceptable to the major parties involved (Congress, the President's Office of Management and Budget, the administering agency, other federal agencies affected, cities and states where appropriate, major public interest groups, etc.). If opposition can be anticipated, the policy should be so clearly in the public interest that the opposition can likely be overcome.

Legal aspects of the policy. The envisaged programme should not be susceptible to legal challenge. In the event that it is (and assuming objections are not constitutional in nature), what enabling legislation would be required, and what specific statutory provision would minimize the susceptibility to litigation of the envisaged policy or programme?

Target population support of the policy. There should be good reasons to believe that the proposed policies will receive strong support in the target groups and provoke the desired response in these groups, i.e., promote innovation.

Cost acceptability of the policy. Assuming successful experimental results, the subsequent policy recommendation should fall within acceptable federal budget limitations.

Effectiveness and range of the policy. The envisaged policy or programme needs to be effective. An effective policy or programme would be one which can reasonably be expected to induce decisively more of the kind of innovation desired, and to apply to a broad range of situations.

Equity of the policy. The envisaged policy or programme should appear equitable to knowledgeable observers. In the first and most important sense, equitable programmes should recognize that fair treatment is central to success. For example, a programme to aid inventors would require uniform selection standards applicable to all inventors. However, this may come into conflict with other objectives (e.g., to give priority to a particular kind of inventor of technology).

Understanding of the policy. The envisaged programme needs to be communicable. Effective administration of public policies and programmes requires that the provisions and requirement; involved be readily communicable to all parties concerned - for example, to legislators, to federal officials, members of regulatory commissions, innovators, and the public at large.

Administration of the policy. The envisaged policy or programme must be able to be carried out without requiring excessive administrative inputs by the federal government. (Administrative inputs are a special class of costs.)

Monitoring of the policy. The agency that is to monitor the effects of the proposed policy should be able to do so with readily available management information. In particular, how can programme performance be monitored; what are the information requirements for evaluating progress; etc.?

Organizational structure to implement the policy. What sort of organizational structure is needed to carry out the programme? Does it exist? Can it be brought into being? Where a programme is to be carried out by an existing governmental agency is the quality of management up to the task?

Sound experimental hypothesis. The most carefully planned experiment will not compensate for the lack of a sound hypothesis. The hypothesis being tested should have antecedents in an explicit or implicit model of the innovation process. Without such conceptual ties, experimental hypotheses lack legitimacy and bring experimental design into serious question. The experimental results should be fed back to the model from which the hypothesis was derived, either to substantiate the model's continued viability or to require its modification.

Careful experimental design. The conceptual and technical design of the experiment must adhere to recognized social science research standards. The dependent, independent and parametric variables must be identified, specified and the relationships among them sorted out so as to present a logical and internally consistent proposition, or set of propositions. The subject population should be identified in terms of quantities and characteristics. A procedure should be developed dealing with the necessity of a control group, the sample sizes needed, the method of sample selection, and the statistical operations to be performed on the indicator measures so as to arrive at significant conclusions. The results of the experiment should be unambiguous in interpretation, free from bias introduced by the experiment itself, and determined with a desired degree of precision. Finally, the experimental design should be as efficient as possible in terms of experimental effort expended.

Feasibility of the experiment. It must be possible to conduct an adequate experiment that requires the availability of a data base, the development of adequate controls, sufficient sample size (where appropriate) to assure necessary statistical reliability, and output measures that reflect the effects of the treatment or intervention.

Time scale of the experiments. The duration of the experiments must be sufficiently short so that the results can be utilized in setting policy, not merely evaluating policy decisions already taken.

Cost of the experiment. The cost of the experimental programme must be less than the perceived value of the information expected to result from it. That value should be estimated at the probable excess cost resulting from a policy decision made with inadequate information.

Cost-effectiveness of the experiments. The envisaged experiment should be the most cost-effective way of obtaining the information needed for the design of a larger-scale government policy or programme. A comparison with other possible means of obtaining the needed information (e.g., case studies of past programmes, surveys, simulation) should underlie the cost-effectiveness decision not compensate for the lack of a sound hypothesis. The hypothesis being tested should have antecedents in an explicit or implicit model of the innovation process. Without such conceptual ties, experimental hypotheses lack legitimacy and bring experimental design into serious question. The experimental results should be fed back to the model from which the hypothesis was derived, either to substantiate the model's continued viability or to require its modification.

Conclusions

The analysis of calculators, analysers, information, expert and decision support systems, neural networks that were developed by researchers from various countries assisted the authors to create of their own Decision Support Web-Based System for Innovation (*IDSS*). *IDSS* differ from others in the use of new multiple criteria analysis methods as were developed by the authors. The database of a best practices were developed providing a comprehensive assessment of alternative versions from the economic, technical, technological, management, organizational, qualitative, legislative and other perspectives. Based on the above complex databases, the developed System enables the user to analyse innovation alternatives quantitatively (i.e. a system and subsystems of criteria, units of measure, values and weights) and conceptually (i.e. the text, formula, schemes, graphs, diagrams and videotapes). A survey of innovation technologies in construction has been made using recent developments in information technology and the opportunities provided by the Internet (i.e. analysers, software applications, websites). The information found mainly refers to the ways of increasing innovation transfer to provide information about new products and processes to users. The influence of information is often assessed from social, economic, technical and other perspectives.

According to the data obtained, the Government should support the development of nanotechnology as the most rational of all the alternatives considered under the initial conditions. The calculations show that the use of nanotechnology in construction is the most rational option to be supported by the government. However, the economic state of the country is not favourable for making huge investments into a new branch. It is not possible because the financial resources are highly limited.

References

[1] Tomala F., Sénéchal O. (2004) Innovation Management: a synthesis of academic and industrial points of view, *International Journal of Project Management*, **22**, No. 4, pp.281-287.

[2] Kaklauskas A., Zavadskas E. (2002) *Web-Based Decision Support.* Vilnius: Technika. 296 p.

[3] Zavadskas E.K., Kaklauskas A., Lepkova N., Gikys M., Banaitis A. (2002) Web-Based Simulation System for Facilities Management. In: *S'02 - SCM Conference*, *Poland, October 23-25, 2002*, pp.515-522

[4] Zavadskas E.K., Kaklauskas A., Trinkunas V. (2002) Increase of efficiency of construction materials e-commerce systems applying intelligent agents. In: *ConstructionInnovation and Global Competitiveness. 10th International Symposium. September 9-13, 2002. Cincinnati, USA.*

[5] Robbins D.M., Milliken G.J. *Government Polices for Technological Innovation: criteria for an experimental approach.* Denver, Colorado 80208, USA: University of Denver, Denver Research, pp. 215-240.

[6] Zavadskas E.K., Simanauskas L., Kaklauskas A. (1998) *Sprendimų paramos sistemos statyboje*. Vilnius: Technika. 235 p.

[7] Завадскас Э.К. (1997) *Комплексная оценка и выбор ресурсо – сберегающих решений в строительстве.* Вильнюс.

[8] Kvederytė N., Zavadskas E.K., Kaklauskas A. (2000) Vienbučių gyvenamųjų namų gyvavimo proceso daugiakriterinė analizė, *Statyba*, **6**, No 3.

[9] http://www.pathenet.org

[10] http://www.mainroad.qid.gov.au

[11] http://www.fgcu.edu/cob/iti/iti.html

[12] http://ims.org/projects/outlina/cumap.html

[13] http://www.eriknetwork.net/

[14] www.egip.com

[15] http://www.europa.eu.int/comm/regional_policy/innovation/innovating/bic_en.html

Received on the 21st of May 2005

Computer Modelling and New Technologies, 2005, Vol.9, No.1, 68-72
Transport and Telecommunication Institute, Lomonosov 1, LV-1019, Riga, Latvia

THE SYNTHESIS OF OPTIMAL CONTROL IN THE VEHICLE SUSPENSION AND IT'S TECHNICAL REALIZATION

V. SHARAPOV

Baltic Russian Institute
3 Piedrujas str, Riga, LV-1073, Latvia

The problem of the optimal regulation of the vehicle suspense synthesis has been solved. The solution is based on the optimal filtration theory of Kolmogorov-Viner.

We consider such regulation of the suspended object to be optimal which provides the required minimum of vibrations under the minimal power consumption of the regulation system. The law found for the regulation of the back communication circuit states that the closed system "object-regulation" is stable and optimal in the sense of the selected criteria of quality.

A simplified form of the optimal regulation law has been suggested; it permits technical realization, using widely known means of automatics.

Keywords: *Kolmogorov-Viner optimal filtration theory, vehicle*

Consider that the motion of an object to be isolated is described by a linear differential equation with constant coefficients

$$P(s)\cdot z(t)=M(s)\cdot u(t)+L(s)\cdot z_g(t), \tag{1}$$

where
$z(t)$ - the object coordinate; $u(t)$ - the controller coordinate; $z_g(t)$ - the external disturbance (micro profile of the road); $P(s), M(s), L(s)$ - the operators of polynomials $s=d/dt$.

The controller coordinate $u(t)$ is defined as its force factor, since at the known disturbance $z_g(t)$ and ride characteristic specified by the accelerations function

$$x(t)=s^2\cdot z(t) \tag{2}$$

any scheme of the suspension controllers of the vehicle would have an approximately same value of the velocity factor. Under existing conditions, the force factor $u(t)$ of the regulator determines its power efficiency.

Thus, we have to determine the law of control in the feedback loop (or, to obtain a differential equation connecting $u(t)$ and $z(t)$) so that the closed-loop control system "object + controller" (1) would be stable and optimal in terms of the minimum quadratic function

$$I=r\cdot m^2\langle x^2\rangle+\lambda\langle u^2\rangle, \tag{3}$$

where $\langle x^2\rangle, \langle u^2\rangle$ - dispersions $x(t)$ and $u(t)$; r, λ - the weighting constants; m - the dimensional coefficient – in this particular case may be equal to the mass of the isolated object.

In other words, it is necessary to obtain the equation of the controller

$$u(t)=W(s)\cdot z(t), \tag{4}$$

where $W(s)$ is the sought transfer function, such as for the function (3) to attain minimum in the class of stable closed-loop systems "object + controller".

Let's use the Fourier transformation (assuming that $s = j\omega$) and express function (3) as

$$I = \frac{1}{i}\int_{-i\infty}^{i\infty} \frac{\left[rm^2 s^4 + \lambda \cdot W(s)\cdot W(-s)\right]\cdot L(s)\cdot L(-s)\cdot S_g(s)}{\left[P(s)-M(s)\cdot W(s)\right]\left[P(-s)-M(-s)\cdot W(-s)\right]}ds \ , \tag{5}$$

where $S_g(s) = S_1(s)\cdot S(-s)$ is the spectral density function of the road micro profile.

One of the possible methods of finding a solution in the class of functions, without upsetting the stability of the closed-loop system (1), is the method [1] of choosing the variable function in the format

$$\Phi_1(s) = \frac{s^2 \cdot L(s)}{P(s)-M(s)\cdot W(s)} \ . \tag{6}$$

In this case, function (5) becomes quadratic in respect to $\Phi_1(s)$.

$$\begin{aligned} I = \frac{1}{i}\int_{-i\infty}^{i\infty} \Big\{ &\left[rm^2 s^4 M(s)\cdot M(-s) - \lambda P(s)\cdot P(-s)\right]\cdot \Phi_1(s)\cdot \Phi_1(-s) - \\ &- \lambda\left[s^2\Phi_1(s)\cdot P(s)\cdot L(-s) + s^2\Phi_1(-s)\cdot P(-s)\cdot L(s) - s^4 L(s)\cdot L(-s)\right]\Big\}\times \frac{S_g(s)}{s^4 M(s)\cdot M(-s)}ds \ , \end{aligned} \tag{7}$$

Let's write the expression for the first variation of that function

$$\begin{aligned} \delta I = \frac{1}{i}\int_{-i\infty}^{i\infty} \Bigg\{ &\left[rm^2 s^4 M(s)\cdot M(-s) + \lambda P(s)\cdot P(-s)\right]\frac{S_g(s)\cdot \Phi_1(s)}{s^4 M(s)\cdot M(-s)} - \\ &- \lambda s^2 P(-s)\cdot L(s)\frac{S_g(s)}{s^4 M(s)\cdot M(-s)}\Bigg\}\delta\Phi_1(-s)\cdot ds + \\ + \frac{1}{i}\int_{-i\infty}^{i\infty} \Bigg\{ &\left[rm^2 s^4 M(s)\cdot M(-s) + \lambda P(s)\cdot P(-s)\right]\frac{S_g(s)\cdot \Phi_1(-s)}{s^4 M(s)\cdot M(-s)} - \\ &- \lambda s^2 P(s)\cdot P(-s)\frac{S_g(s)}{s^4 M(s)\cdot M(-s)}\Bigg\}\delta\Phi_1(s)\cdot ds \ . \end{aligned} \tag{8}$$

In accordance with the solution procedure for the Wiener-Hopf equation [1] let's implement the following intermediate transformations in integral (8). The multiplier of the function $\Phi_1(s)$ can be presented as a product of two functions.

$$\left[rm^2 s^4 M(s)\cdot M(-s) + \lambda P(s)\cdot P(-s)\right]\cdot \frac{S_g(s)}{s^4 M(s)\cdot M(-s)} = D_1(s)\cdot D(-s) \ , \tag{9}$$

where $D_1(s)$ has the zeroes and poles only on the left half-plane s (LHP).

Let's also present

$$\frac{\lambda}{D_1(-s)}\cdot s^2 \cdot P(-s)\cdot L(s)\cdot \frac{S_g(s)}{s^4 M(s)\cdot M(-s)} = B_{10}(s) + B_{1+}(s) + B_{1-}(s) \ , \tag{10}$$

where $B_{10}(s)$ is a polynomial from s; $B_{1+}(s)$ is a regular polynomial fraction with poles only in LHP; $B_{1-}(s)$ is a regular polynomial fraction with poles only in RHP.

Using assumed symbols, the expression for the first variation of the functional may be expressed as follows

$$\delta I = \frac{1}{i}\int_{-i\infty}^{i\infty} D_1(-s)\left[D_1(s)\Phi_1(s) - B_{10}(s) - B_{1+}(s) - B_{1-}(s)\right]\delta\Phi_1(-s)ds + \\ + \frac{1}{i}\int_{-i\infty}^{i\infty} D_1(s)\left[D_1(-s)\Phi_1(-s) - B_{10}(-s) - B_{1+}(-s) - B_{1-}(-s)\right]\delta\Phi_1(s)ds . \quad (11)$$

Then the function $\Phi_1(s)$, setting to zero the first variation of function δI and having poles only in LHP is defined by the expression

$$\Phi_1(s) = \frac{1}{D_1(s)}\left[B_{10}(s) + B_{1+}(s)\right] . \quad (12)$$

Having determined $\Phi_1(s)$ as (12), from (6) we find the expression of the sought transfer function

$$W(s) = \frac{\Phi_1(s)\cdot P(s) - s^2 L(s)}{\Phi_1(s)\cdot M(s)} . \quad (13)$$

In [1] it is proved that if the initial control object is stable, then the closed-loop control system "object + controller" with the feedback loop described by (13) will also be stable.

For the elementary suspension system (Figure 1)

$$\begin{cases} P(s) = ms^2 + bs + c ; \\ M(s) = 1 ; \\ L(s) = bs + c ; \end{cases} \quad (14)$$

where m -is the mass of suspended body; b is the coefficient of viscous damping; c is the stiffness of a spring.

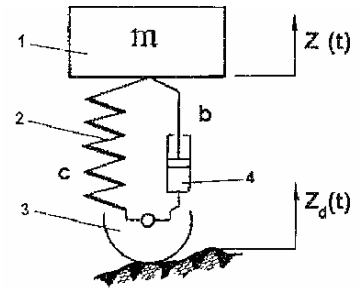


Figure 1. The simplest single-supported scheme of transportation means for research suspension: 1- sprung body or frame of vehicle; 2- spring of suspension; 3- wheel of a vehicle; 4- shock absorber of suspension; Z(t) – the vertical coordinate of sprung body; $Z_d(t)$ – the external disturbance (micro profile of the road)

Considering (14), expression (12) for the function being varied after simple transformations becomes

$$\Phi_1(s) = \frac{s^4(bs + c)}{\left(ms^2 + bs + c\right) + \frac{r}{\lambda}\cdot\frac{m^2 s^4}{\left(ms^2 - bs + c\right)}} . \quad (15)$$

The desired optimal control may be presented as

$$W(s) = -\frac{r}{\lambda}\cdot\frac{m^2 s^4}{ms^2 - bs + c} . \quad (16)$$

The weighting constants r and λ may have different values but their sum stay the same, in this particular case, equal to unity. The ratio of the weighting constant in (10) has the meaning of the gain of the control system and is designated as

$$k = \frac{r}{\lambda} . \quad (17)$$

If we are satisfied with the ride quality ensured by the installed suspension, or we can't allow an additional energy consumption to improve ride quality, then $r = 0$, $\lambda = 1$, $k = 0$, that is, no control. In this case we have a regular passive vibration isolation system.

If it is necessary to increase the ride quality regardless of energy consumption considerations, then $\boldsymbol{r \to 1}$, $\lambda \to 0$ and $k \to \infty$. In real conditions $\lambda \neq 0$ always; therefore gain k has a finite value, determined by a stability margin and the power of the energy source for the controller.

The analysis of the expression (16) leads to the conclusion that the control hardware is very complicated. Really, for the control law (16) the fourth derivative of the suspended mass displacement is essential, as well as the first and second derivatives of the force factor of the controller. However, the experience in control design [2] shows, that obtaining even the second derivative of the object coordinate is very difficult, not to mention the derivatives of a higher order.

Therefore expression (16) for the function of optimal control, taking into account the difficulties of realization, must be considerably simplified.

In expression (16) let's separate the integral (whole) part,

$$W(s) = k\left[ms^2 + bs + \left(\frac{b^2}{m} - c \right) + R(s) \right] , \tag{18}$$

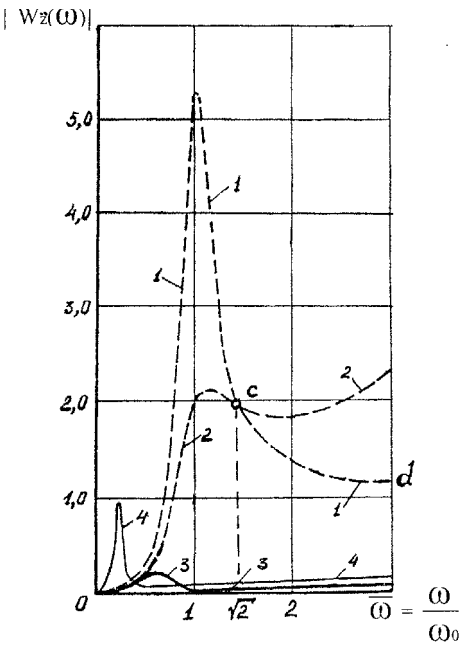
where $R(s) = \dfrac{\left(\dfrac{b^2}{m} - 2bc \right) \cdot s - c\left(\dfrac{b^2}{m} - c \right)}{\left(ms^2 - bs + c \right)}$.

The proper fraction $R(s)$ in the vicinity of the origin can be expanded into the Taylor series, in which only the first two terms will be retained:

$$R(s) = R(0) + R'(0) \cdot s + \dots . \tag{19}$$

Considering that $R(0) = -\left(\dfrac{b^2}{m} - c \right)$; $R'(0) = -b$ and substituting (19) to (18), we will have

$$W(s) \approx W_p(s) = -kms^2 , \tag{20}$$



where $W_p(s)$ is reasonably close to the optimal control function and is adopted for instrumental realization in hardware.

The amplitude-frequency characteristic (AFC) of accelerations of system (14) is presented in Figure 2. Lines 1 and 2 correspond to $k = 0$ (suspension is passive); line 3 represents theoretically optimal control (16), and line 4 represent practically realizable control under the law expressed in (20).

Figure 2. Amplitude-frequency characteristic of sprung body accelerations of some suspensions scheme in the dimensionless form

It's obvious that the optimal control (16) would allow the smoothest ride of the vehicle, but its realization is limited by serious technical difficulties.

The simplified optimal control strategy presented in (20) is equivalent to a reduction in stiffness. The resonance in AFC moves to the left and the natural frequency of system (14) decreases in $\sqrt{k+1}$ times. Thus, if we exclude from consideration the low frequency range (less than 0,3 Hz) of road disturbances the control under (20) is competitive with the theoretically optimal (16) and can provide a radical increase in ride smoothness interest (0,5 – 3,0 Hz).

References

[1] Aliev F.A., Larin V.B., Naumenko K.I. , Suncov V.N. (1978) *Optimization of the Invariant Respect to Time Control Systems.* Kiev: Naukova Dumka. 430 p.
[2] Bessekerski V.A., Popov E.P. (1975) *The Theory of Automatic Control.* Moscow: Nauka. 767 p.
[3] *System Road-Tire-Automobile-Drive Dynamics* / Edited by A.A Khachaturov. Moscow: Mashinostroienie, 1978. 847 p.
[4] *Cert. of Inv. 500992 (USSR).* The Method of Stabilization of the Dynamic Forces Acting Through the Suspension to the Body of the Vehicle.
[5] Sharapov V.D. (1980) *Active Suspensions of Vehicles.* Riga. 226 p.

Received on the 21st of May 2005

Computer Modelling & New Technologies, 2004, Volume 9, No.1
Transport and Telecommunication Institute, Lomonosov Str.1, Riga, LV-1019, Latvia

Authors' index

Yuri N. Shunin (b. March 6, 1951 in Riga)

- Vice-rector on innovation work (Information Systems Management Institute), professor, Dr.Sc. Habil.
- *Director of specialities*: Semiconductor Electronics & Technologies, Computer simulation of semiconductor technologies (Transport and Telecommunication Institute, Riga).,
- *Director of speciality:* Information Systems (Information Systems Management Institute).
- **University study**: Moscow physical and technical institute (1968-1974).
- Ph.D. (physics & mathematics) on solid state physics (1982, Physics Institute of Latvian Academy of Sciences), Dr. Sc. Habil (physics & mathematics) on solid state physics (1992, Ioffe Physical Institute of Russian Academy of Sciences).
- **Publications:** 290 publications, 1 patent.
- **Scientific activities**: solid state physics, physics of disordered condensed media, amorphous semiconductors and glassy metals, semiconductor technologies, heavy ion induced excitations in solids, mathematical and computer modelling, system analysis

Igor V. Kabashkin (born in Riga, 1954)

- Vice-rector for Research and Development Affairs of Transport and Telecommunication Institute, Professor, Director of Telematics and Logistics Institute,
- PhD in Aviation (1981, Moscow Institute of Civil Aviation Engineering), Dr.Sc.Habil. in Aviation (1992, Riga Aviation University), Member of the International Telecommunication Academy, Member of IEEE, Corresponding Member of Latvian Academy of Sciences (1998)
- **Publications:** 320 scientific papers and 67 patents.
- **Research activities:** information technology applications, operations research, electronics and telecommunication, analysis and modelling of complex systems, transport telematics and logistics

Marina Kopeetsky

- received B.Sc. degree in mathematics in 1987 at St. Petersburg University of Education, Russia;
- received M.Sc. and Ph.D. degrees in Computer Science and Mathematics at Bar-Ilan University, Israel in 1997 and 2002, respectively;
- scientific interests include mathematical modelling and optimization of Computer Communications [protocols, continual computations methods and fault tolerant computer systems design.

S,M. Lyubkin, Dc.Sc., Dozent

The Member of Russian Project Management Association Council

Professional interests: Hierarchic Project Management

V.S. Rezer, Dr.Sc.

The Member of Russian Project Management Association

Professional interests: Investment project management

A. Ben-Yair

Post-graduate student of University of Ben-Gurion of Negev, Israel

Professional interests: Economical aspects of reliability, planning net-project management

A.V. Malisheva

Post-graduate student of University of Ben-Gurion of Negev, Israel

Professional interests: Economical aspects of reliability, planning net-project management

A.I. Kravchenko, Dr.Sc.

The Member of Russian Project Management Association

Professional interests: project management

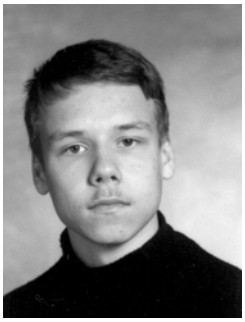
Angelika Strutz

Post-graduate student of University of Ben-Gurion of Negev, Israel

Scientific interests*:* Phase transitions in metal alloys and compounds, structure of solids, diffusion processes in solids, computer modelling in materials science.

David Fuks (b. December, 1948, Odessa, Ukraine)

Professor, Dr. Sc. Habil. Prof. of the Department of Materials Engineering of the Ben-Gurion University of the Negev (Israel).
University study: Mechnikov Odessa State University, Department of Theoretical Physics, 1971
Publications: One book, six chapters in collective volumes and more than 200 papers.
Scientific interests*:* Phase transitions in metal alloys and compounds, structure of solids, diffusion processes in solids, computer modelling in materials science.



Alex Gopeyenko, BSc

Information Systems Management Institute (2005)

Scientific interests**:** solid state physics calculations and modelling

Edmundas Kazimieras ZAVADSKAS, Doctor Habil, Professor, Dr honoris causa multi, Vice-Rector of Vilnius Gediminas Technical University. Member of Lithuanian Academy of Sciences, President of Lithuanian Operational Research Society, President of Alliance of Experts of projects and buildings of Lithuania.

In 1973 Doctor of Science (building structures). Professor at the Department of Construction Technology and Management. In 1987, Dr Habil degree (problems of building technology and management). Research visits to Moscow Civil Engineering Institute, Leipzig and Aachen Higher Technical Schools. He maintains close academic links with the universities of Aalborg (Denmark), Salford and Glamorgan (UK), Poznan University of Technology (Poland), Leipzig Higher School of Technology, Economics and Culture (Germany). Member of international organizations. Member of steering and programme committees of many international conferences. Member of editorial boards of some research journals. Author of monographs in Lithuanian, English, German and Russian.
Research interests: building technology and management, decision-making theory, automation in design, expert systems.

Arturas KAKLAUSKAS. Doctor Habil, Professor, Department of Construction Economics and Property Management, Vilnius Gediminas Technical University (VGTU), Saulėtekio al. 11, LT-10223 Vilnius, Lithuania.

Academic Experience (Vilnius Gediminas Technical University): PhD Student (1987-1989), Senior lecturer (1990-1995), Associate Professor (1995-2000), Chairman of the Department of Construction Technology and Management (1996-2001), professor (2000), Chairman of the Department of Construction Economics and Property Management (2001). A. Kaklauskas participates in four Framework 5 programs and is the leader of the CIB Study group SG1 "The Application of Internet Technologies in Building Economics".

Research interests: Internet based and e-business systems (property, construction and export), decision making theory, decision support systems, etc. Publications: Author of 87 scientific articles and 5 monographs.

CUMULATIVE INDEX

COMPUTER MODELLING and NEW TECHNOLOGIES, volume 9, No. 1, 2005 (Abstracts)

A. Strutz, D. Fuks. Amphoteric Properties of Cr in FeAl(B2) Phase, *Computer Modelling and New Technologies,* vol. 9, No 1, 2005, pp. 7–14.

The study of the influence of the vacancy on the Fe site and alloying by Cr on the band structure of the FeAl phase with the vacancy is performed on the basis of the Full Potential Augmented Plane-Wave (APW) + Local Orbitals (LO) method with WIEN 2k package. The changes in the total and the partial Densities of States (DOS), as a result of vacancy formation and alloying by Cr, are obtained and discussed. The formation of the "pocket" in the electron density in the vicinity of vacancy is revealed. We found that formation of the vacancy on the iron site leads to significant increase of the main peak in total DOS just below the Fermi energy together with the corresponding narrowing of the bands located below the Fermi level. The analysis shows that the formation of the vacancy on the Fe site leads to the creation of the damping wave of electronic excitations. Comparison of the partial DOS for d-electrons for different iron atoms in the extended cell clearly shows that this is the excitation of mainly d-states that reveal the same tendency as the total on-site DOS. At the same time the partial DOS for p-states for Al atoms does not show any noticeable change when the vacancy on the Fe site is formed. We found the changes in the site preference for Cr substituting for Fe or Al when the vacancy in FeAl(B2) phase is formed. The bonding tendencies and the changes in DOS in this case are discussed.

Keywords*: Fe-Cr, FeAl alloys, WIEN 2k package, Augmented Plane-Wave + Local Orbitals* (*APW+LO), Densities of States*

Yu.N. Shunin, A.V. Gopeyenko. Phase-shift Functions Method for Nanoclusters Electronic Structure Calculations in Solids, *Computer Modelling and New Technologies,* vol. 9, No 1, 2005, pp. 15–31.

Presently in semiconductor technologies at the micrometer length scale is being used. However, these technologies have achieved the physical limits. Now the downscaling of semiconductor devices to a new technology at the nanometer length scale is expected. Successful production of nanometer scale devices requires a clear understanding of physical and electronic properties of nanometer scale systems.

Nanoclusters have a wide range of applications that depend on their properties. Different kinds of materials are used in different areas. For example metals that have magnetic properties (such as Fe, Cu) can be used for development of new high-density storage devices. Si and Ge are used in semiconductor technologies to produce different nanometer scale electronic devices.

There is a considerable interest in the geometrical, electronic, and chemical properties of nanoscale clusters. Such clusters represent an intermediate phase of matter, whose material properties are often quite different from either the single-atom or bulk properties of the elements involved. With the current scientific focus on nanotechnology, the field of cluster research has received renewed impetus, as clusters may well provide suitable building blocks for the construction of desirable nanostructures. It is in this context that the quantum transport properties of nanoscale clusters may well prove to be important. The recent advent of molecular electronic systems has opened up a frontier in which atoms, clusters, and/or molecules assume the role of electronic device elements. A progress in this field has been rapid, and already prototypical molecular logic circuits have been constructed in laboratories. However, there are many outstanding problems, which need to be understood. In particular, solid-state calculations for nanoobjects are actually. The main attention in this work is paid to the electronic scattering calculation for atomic clusters, which are the nanobjects.

Keywords*: nanotechnology, nanocluster, Shrödinger equation, phase function, phase shift, potential, tight binding approximation (TBA), nearly free electron approximation (NFEA)*

M. Kopeetsky. Mathematical Modelling of the Wireless Communication Network*, Computer Modelling and New Technologies,* vol. 9, No 1, 2005, pp. 32–39.

The paper is devoted to study and evaluation of the erroneous packets flow on the physical layer of a wireless communication network. A mathematical model of the erroneous packets passed to the communication channel has been structured and analysed. The statistical estimation of the erroneous packets number is presented and discussed in the paper.

Keywords*: Wireless communication channel, erroneous packets, error bursts.*

Z. Laslo, D. Golenko-Ginzburg, A. Gonik. Alternative Stochastic Network Projects with Renewable Resources, *Computer Modelling and New Technologies,* vol. 9, No 1, 2005, pp. 40–46.

The paper presents a heuristic for resource constrained network project scheduling. A network project comprising both alternative deterministic decision nodes and alternative branching nodes with probabilistic outcomes is considered. Several renewable activities related resources, such as machines and manpower, are imbedded in the model. Each type of resources is in limited supply with a resource limit that is fixed at the same level throughout the project duration. Each activity in the project requires resources of various types with fixed capacities. The activity duration is a random variable with given density function. The problem is to minimize the expected project duration by determining for each activity, which will be realized within the project's realization, its starting time (decision variable), i.e., the time of feeding-in resources. The resource delivery schedule is not calculated in advance and is based on decision-making in the course of monitoring the project. The suggested heuristic algorithm is performed in real time via simulation. Decision-making is carried out:

- at alternative deterministic decision nodes, to single out all the alternative subnetworks (joint variants) in order to choose the one with the minimal average duration;
- at other essential moments when at least one activity is ready to be operated but the available amount of resources is limited. A competition among those activities is carried out to determine the subset of activities which have to be operated first and can be supplied by available resources. Such a competition is realized by a combination of a knapsack resource reallocation model and a subsidiary simulation algorithm.

Keywords*: Alternative decision nodes, probabilistic branching, joint variant, renewable resources, resource constrained GERT project scheduling algorithm, stochastic project simulation*

A.I. Kravchenko, S.M. Lyubkin, V.S. Rezer, A. Ben-Yair, A.V. Malisheva. Distribution Algorithms of the Valueing Resources at Design Office, *Computer Modelling and New Technologies,* vol. 9, No 1, 2005, pp. 47–56.

At formation of the summary thematic plan of design office for the certain scheduled period the task of the budget optimum distribution, allocated for this period, between the separate projects is considered. The generalized parameter including a degree of a priority on each project, probability of performance of the project to prognosticated term, which is determined during the decision of a task, is taken into account as optimality criterion. The displacement value of this term respectively given one is also defined. The solution of a task is based on the dynamic programming method use.

Keywords*: budget optimum distribution, design office, dynamic programming*

E.K. Zavadskas, A. Kaklauskas, M. Viteikiene. Decision Support Web-based System for Construction Innovation, *Computer Modelling and New Technologies,* vol. 9, No 1, 2005, pp. 57–67.

Many construction and facilities management Web sites can be found on the Internet. The interested parties on construction and facilities management Web sites can find databases of best practices, analysers, software, expert and decision, etc.

Technological innovation mainly through changes in the availability of information and communication technology inclusive databases of best practices, calculators, analysers, software,

neural networks, decision support and expert systems that have been provided by a variety of new services developed by the construction and facilities management sectors.

Most of all calculators, analysers, software, decision support and expert systems, neural networks and on-line systems seek to find out how to make the most economic decisions and most of all these decisions are intended only for economic objectives. Alternatives under evaluation have to be evaluated not only from the economic position, but take into consideration qualitative, technical, technological and other characteristics as well. Based on the analysis of the existing calculators, analysers, information, expert and decision support systems, neural networks and in order to determine most efficient versions of best practices a Decision Support Web-Based System for Construction Innovation (IDSS) was developed by Vilnius Gediminas Technical University.

Innovation activities involve a number of interested parties who pursue various goals and have different potentialities, educational levels and experiences. This leads to various approaches of the above parties to decision-making in this field. In order to do a full analysis of the available alternatives and to obtain an efficient compromise solution, it is often necessary to analyze economic, technical, technological, management, organization, legal, social and other information. This information should be provided in a user-oriented way.

Keywords*: construction, innovation, decision support system, multiple criteria*

V. Sharapov. The Synthesis of Optimal Control In The Vehicle Suspension And It's Technical Realization**,** *Computer Modelling and New Technologies,* vol. 9, No 1, 2005, pp. 68–72.

The problem of the optimal regulation of the vehicle suspense synthesis has been solved. The solution is based on the optimal filtration theory of Kolmogorov-Viner.

We consider such regulation of the suspended object to be optimal which provides the required minimum of vibrations under the minimal power consumption of the regulation system. The law found for the regulation of the back communication circuit states that the closed system "object-regulation" is stable and optimal in the sense of the selected criteria of quality.

A simplified form of the optimal regulation law has been suggested; it permits technical realization, using widely known means of automatics.

Keywords*: Kolmogorov-Viner optimal filtration theory, vehicle*

COMPUTER MODELLING and NEW TECHNOLOGIES, 9.sējums, Nr.1, 2005

(Anotācijas)

A. Strutz, D. Fuks. *Cr amfotēriskās īpašības FeAl(B2) fāzē, Computer Modelling and New Technologies,* 9.sēj., Nr.1, 2005, 7.–14. lpp.

Pētījums par Fe izvietojuma vakances ietekmi un par Cr sakausējumu uz FeAL fāzes joslas struktūras ar vakanci ir veikts, pamatojoties uz *Full* Potential *Augmented Plane-Wave (APW) + Local Orbitals (LO)* metodi ar *WIEN 2k* paketi. Darbā ir iegūtas un diskutētas izmaiņas totālā un parciālā stāvokļa blīvumā - *Densities of States* (DOS), kas ir kā vakances veidošanās un Cr sakausējuma rezultāts. Ir parādīta "kabatas" veidošanās elektronu blīvumā vakances apkārtnē.

Autori konstatēja, ka vakances veidošanās uz dzelzs rada nozīmīgu palielinājumu totālās *DOS* galvenajā smailē tieši zem *Fermi* enerģijas kopā ar atbilstošo joslu sašaurinājumu, kas izvietotas zem *Fermi* līmeņa. Analīze parāda, ka vakances veidošanās uz dzelzs noved pie elektronisko svārstību viļņu noslāpējuma rašanās.

Savienojuma tendences un izmaiņas *DOS* rakstā tiek iztirzātas.

Atslēgvārdi*: Fe-Cr, FeAL sakausējumi, WIEN 2k paketes, Augmented Plane-Wave + Local Orbitals* (*APW+LO), stāvokļa blīvums - Densities of States (DOS)*

YU.N. Shunin, A.V. Gopeyenko. Fāzes nobīdes funkciju metode nanoklasteru elektronisko struktūru aprēķiniem cietvielās, *Computer Modelling and New Technologies,* 9.sēj., Nr.1, 2005, 15.–31. lpp.

Pašlaik pusvadītāju tehnoloģijas tiek pielietotas mikrometru garuma mērogos. Tomēr šīs tehnoloģijas ir sasniegušas fiziskās robežas. Pašlaik ir paredzēta pusvadītāju ierīču izmēru samazināšanās saskaņā ar jaunām nanometru garuma mēroga tehnoloģijām.

Nanoklasteriem ir plaša mēroga pielietojums, kas ir atkarīgs no to īpašībām. Tiek lietoti dažādi materiāli dažādās vietās. Piemēram, metāli, kuriem ir magnētiskās īpašības (Fe, Cu), var tikt pielietoti, lai izveidotu jaunas izteikta blīvuma ierīces. Si un Ge tiek lietots pusvadītāju tehnoloģijās, lai ražotu dažādas nanometru mēroga elektroniskās ierīces. Pastāv arī vērā ņemama interese ģeometrisko, elektronisko un ķīmisko īpašību izmantošanā nanomēroga klasteros.

Šajā sfērā tiek sasniegts ļoti ātrs progress, līdz ar to laboratorijās ir jau izveidotas prototipu molekulārās loģiskās ķēdes. Šajā darbā ir veikti elektroniskās izkliedes aprēķini atomu klasteriem, kuri ir nanoobjekti.

Atslēgvārdi*: nanotehnoloģijas, nanoklasteris, Šrēdingera vienādojums, fāzes funkcija, fāzes nobīde, potenciāls, ciešās saiknes aproksimācija (tight binding approximation - TBA, gandrīz brīvo elektronu aproksimācija (nearly free electron approximation -NFEA)*

M. Kopeetsky. Bezvadu komunikāciju tīkla matemātiskā modelēšana, *Computer Modelling and New Technologies,* 9.sēj., Nr.1, 2005, 32.–39. lpp.

Raksts ir veltīts bezvadu komunikāciju tīkla fiziskā slāņa kļūdaino pakešu plūsmas izpētei un novērtēšanai. Ir izveidots un analizēts kļūdaino pakešu, kas tiek padotas komunikāciju kanālam, matemātiskais modelis. Bez tam rakstā tiek parādīts un diskutēts kļūdaino pakešu skaita statistiskais izvērtējums.

Atslēgvārdi*: bezvadu komunikāciju kanāls, kļūdainās paketes, kļūdu eksplozija*

Z. Laslo, D. Golenko-ginzburg, A. Gonik. Alternatīvie stohastiskie tīkla projekti ar atjaunojamiem resursiem, *Computer Modelling and New Technologies,* 9.sēj., Nr.1, 2005, 40.–46. lpp.

Rakstā tiek prezentēta heiristika jeb jaunatklāsme tīkla resursu projekta sastādīšanā. Tiek izskatīts tīkla projekts, kas iekļauj kā alternatīvo noteicošo lēmumu kopumu, tā arī alternatīvos nozaru mezglus ar varbūtējiem iznākumiem. Modelī ir iekļautas dažas atjaunojamās aktivitātes, kas ir

saistītas ar resursiem, e.g. mehāniskais un cilvēka spēks. Katrs resursu tips ir ierobežotā daudzumā ar resursu limitu, kas tiek fiksēts tajā pašā līmenī visā projekta garumā. Katra aktivitāte projektā pieprasa dažādus resursu tipus ar fiksētām kapacitātēm. Problēma pastāv projekta ilguma minimizēšanā, nosakot katrai aktivitātei, kas tiek īstenota visa projekta realizācijas gaitā, tā sākuma laiku (lēmuma mainīgais), i.e., resursu papildināšanas laiku. Resursu piegādes grafiks netiek aprēķināts uz priekšu, un tas pamatojas uz lēmumu pieņemšanu projekta monitoringa gaitā. Piedāvātais heiristiskais algoritms tiek veikts reālā laikā *via* simulācija.

Atslēgvārdi*: alternatīvais lēmumu kopums, saistītais variants, atjaunojamie resursi, stohastiskā projekta simulācija*

A.I. Kravčenko, S.M. Ļubkin, V.S. Rezer, A. Ben-Jair, A.V. Mališeva, Vērtības resursu sadales algoritmi konstruktoru birojā, *Computer Modelling and New Technologies,* 9.sēj., Nr.1, 2005, 47.–56. lpp.

Šajā rakstā autori izskata optimālās sadales uzdevumu, kur tiek ievērotas budžeta iespējas starp atsevišķiem projektiem, veidojot konstruktoru biroja tematisko plānu noteiktam periodam. Vispārinātais rādītājs kā optimalitātes kritērijs tiek ņemts vērā, iekļaujot katra projekta prioritātes pakāpi, projekta izpildes varbūtību katram prognozējamam termiņam, kurš savukārt tiek noteikts uzdevuma risināšanas gaitā, kā arī šī termiņa nobīdes laika lielumu atbilstoši plānotajam. Šī uzdevumā risināšanas pamatā tiek izmantota dinamiskās programmēšanas metode.

Atslēgvārdi*: budžeta optimuma sadale, konstruktoru birojs, dinamiskā programmēšana*

E.K. Zavadskas, A. Kaklauskas, M. Viteikiene, Inovāciju veidošanas *Web* pamatota lēmumu atbalsta sistēma, *Computer Modelling and New Technologies,* 9.sēj., Nr.1, 2005, 57.–67. lpp.

Internet tīklā var atrast ļoti daudz un dažāda tīmekļa vietnes vadības iespējas un uzbūves. Tīmekļa vietnes vadības iespējās un uzbūvē ieinteresētās puses var atrast labākās datu bāzes, analītiķus, programmas, ekspertus etc.

Tehnoloģiskās inovācijas galvenokārt informācijas pieejamība un komunikāciju tehnoloģija, ietverot labākās izmantojamās datu bāzes, kalkulatorus, analītiķus, programmas, lēmumu atbalstītājus un ekspertu sistēmas un neironu tīklus, tiek nodrošināti ar veselu virkni jauniem servisiem, kurus rada konstrukciju un vadības iespēju sektori.

Pamatojoties uz esošo analītiķu, kalkulatoru, informācijas ekspertu un lēmumu atbalsta sistēmām, kā arī neironu tīkliem, lai noteiktu visefektīvākās versijas vislabākajiem pielietojumiem, Gedimina Viļņas Tehniskajā universitātē tika izstrādāta - *Decision Support Web-Based System for Construction Innovation (IDSS)*.

Atslēgvārdi*: uzbūve, inovācija, lēmumu atbalsta sistēma, multiplie kritēriji*

V. Sharapov. Optimālās kontroles sintēze transporta līdzekļu spriegums un tās tehniskā realizācija, *Computer Modelling and New Technologies,* 9.sēj., Nr.1, 2005, 68.–72. lpp.

Rakstā tiek izskatīta transporta līdzekļu sprieguma problēma un parādīts tās risinājums. Risinājums tiek pamatots uz Kolmogorova-Vinera optimālās filtrācijas teoriju. Šis risinājums nodrošina nepieciešamo vibrāciju minimumu.

Tiek piedāvāta optimālo noregulējumu likumu vienkāršotā forma, tā pieļauj tehnisko realizāciju, pielietojot plaši zināmos automātikas līdzekļus.

Atslēgvārdi: *Kolmogorova-Vinera optimālās filtrācijas teorija, transporta līdzeklis*

COMPUTER MODELLING & NEW TECHNOLOGIES

ISSN 1407-5806 & ISSN 1407-5814(on-line)

THE JOURNAL IS DESIGNED FOR PUBLISHING PAPERS CONCERNING THE FOLLOWING FIELDS OF RESEARCH:

- mathematical and computer modelling
- mathematical methods in natural and engineering sciences
- physical and technical sciences
- computer sciences and technologies
- semiconductor electronics and semiconductor technologies
- aviation and aerospace technologies
- electronics and telecommunication
- navigation and radar systems
- telematics and information technologies
- transport and logistics
- economics and management
- social sciences

Articles can be presented in journal in English (preferably), Russian, German and Latvian (at the option of authors). All articles are reviewed.

Computer Modelling & New Technologies * Preparation of Publications

EDITORIAL CORRESPONDENCE

Transporta un sakaru institūts (Transport and Telecommunication Institute)
Lomonosova iela 1, LV-1019, Riga, Latvia. Phone: (+371)-7100593. Fax: (+371)-7100535
E-mail: journal@tsi.lv, http:// www.tsi.lv

COMPUTER MODELLING AND NEW TECHNOLOGIES, 2005, Vol. 9, No.1

Scientific and research journal of Transport and Telecommunication Institute (Riga, Latvia)
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.

$$E_{int} = \iint \psi^{+}(\mathbf{x})\psi(\mathbf{x})K(\mathbf{x}-\mathbf{x}')(-div\mathbf{P}(\mathbf{x}'))d^3xd^3x', \quad (1)$$

$$K(\mathbf{x}-\mathbf{x}') = C_0 \frac{exp(-\lambda(|\mathbf{x}-\mathbf{x}'|)}{|\mathbf{x}-\mathbf{x}'|}. \quad (2)$$

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.

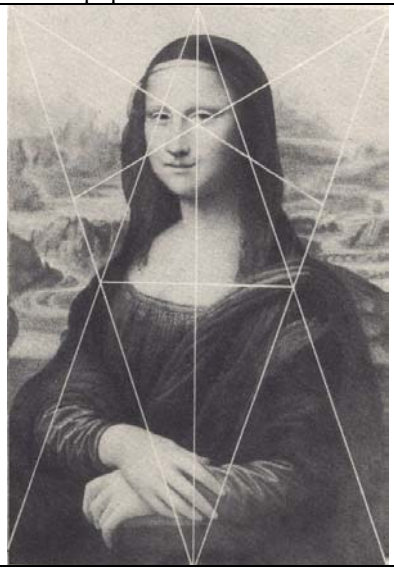
11.1. DISK FORMATS AND WORD PROCESSING PACKAGES

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.

NATURE AND COMPUTER WORLD
Scientific popular journal
ПРИРОДА И КОМПЬЮТЕРНЫЙ МИР
Научно-популярный журнал
DABA UN DATORPASAULE
Zinātniski populārais žurnāls



PUBLISHERS:
TRANSPORT AND TELECOMMUNICATION INSTITUTE
***TRANSPORTA UN SAKARU INSTITŪTS** (TSI)*
&
INFORMATION SYSTEMS INSTITUTE
***INFORMĀCIJAS SISTĒMU AUGSTSKOLA** (ISMA)*

NATURE AND COMPUTER WORLD,
PUBLISHED SINCE 2001
ISSN 1407-8422
ISSN 1407-8422 - **on-line**

Editorial office:
Nature and Computer World,
Lomonosov 1, Build. 4, LV-1019, Riga, Latvia
shunin@tsi.lv, kiv@tsi.lv

N&CW is the new scientific popular journal addressed to senior school students. It pays attention to some actual fields of undergraduate studies:

- Mathematics
- Physics
- Computers
- Programming and Computer Modelling
- Nature Phenomena

We are open for collaboration in these directions in the framework of N&CW and ready to consider corresponding materials. All articles are reviewed.