SUMMARY OF PREVIOUS AND CURRENT RESEARCH INTERESTS

My background covers a broad spectrum of condensed- and soft-matter physics and computational materials physics, particularly processes of pattern formation, nonequilibrium thermodynamic and dynamics of material interfaces. In my research I employ different theoretical methods and computer simulations. A better understanding of the physical mechanisms by which structures are generated in materials is important for practical purposes. Recently my background of a materials physicist found application in another branch of science—biophysics.

MATERIALS PHYSICS

Crystallization. Dendritic Growth. [Ref. 20, 22, 24-30]

The well-known phenomenon of *dendritic* growth is important for crystallization of metals and organic materials from a supercooled melt. The purpose of my dissertation work was *to create the physical model and numerically simulate* different regimes of this phenomenon in conjunction with the large-scale modeling of solidification [24,26]. For the first time the model was able to reproduce the snowflake-like patterns seen experimentally [25,27-30]. The result of this research was twofold. On the one hand, this model allowed us to predict properties of a material obtained in real processing and by choosing the appropriate thermal regime increase the homogeneity of the latter.

On the other hand the model revealed many of the *physical features* pertaining to the growth of a dendrite [25,27]. For example, for the first time the model was able to predict the mechanism of coarsening of the side-branch structure by *period doubling* which was confirmed later by experimental results and provides an important connection with the transition to chaotic structures. Also the model predicts the *restoration of morphological stability* under conditions of rapid solidification, i.e. far from equilibrium. Because of potential importance for applications this effect was analyzed later in the framework of a "string" or geometric model where the interface is viewed as a line of heat sources moving according to the evolution of the diffusion field and in compliance with the natural (geometric) properties of a string. In a strongly supercooled melt, the diffusion field in front of a moving interface is confined to small vicinity and a thermal boundary layer approximation can be introduced. Being applied together with a string model, this approximation allows one to study stability properties of the interface and its dynamics close to the point of absolute morphological stability [20].

Intermetallic Compound Growth. [Ref. 3]

My experience with dendritic solidification recently found an application in a technologically important problem of soldering. When a drop of melt (Sn-based alloy, solder) is brought into contact with a solid Cu-substrate, a layer of intermetallic compound Cu_6Sn_5 starts to grow between the two. Experimental observations demonstrate formation of an intricate microstructure on the surface of the layer, which is interplay of the metal's crystalline properties and dissolution kinetics [3]. My previous theoretical analysis of the intermetallic phase growth highlighted the early stage of soldering as the critical step for the microstructure formation. On the basis of those theoretical ideas I introduced a novel experimental technique, which allowed us to study entire early-stage evolution process on one micrograph. At present in collaboration with NIST I am working on a computer model that will reproduce experimentally observed behavior the intermetallic phase structure [Grants].

Thermal Effects of Phase Transitions. Dynamics of Interfaces. [Ref. 5, 6, 8-13, 15, 17-19, 21, 23, 31]

The solidification problems have stimulated my interest in the physics of interfaces, which are crucial elements of modern sophisticated materials, and dynamics of their motion. Dynamics of interfaces is accompanied by the processes of heat redistribution, which affects the rate and morphology of the evolution in thermodynamic systems. In my early work, using a theoretical approach of a free-boundary problem, a previously unknown regime of interface motion was revealed and verified in numerical simulations [31]. In my later studies, to analyze material's structure on different length scales, I adopted the continuum (phase-field) approach because it allowed me to study time evolution and equilibrium properties on the same basis. In the framework of this method the state of a system undergoing phase transition is characterized by the coarse-grained Hamiltonian (nonequilibrium Ginzburg-Landau free-energy) which, in addition to pressure, temperature and composition, depends upon one more variable, order parameter, that changes continuously from one phase to another [5, 8]. Such parameter has relevance to many different transitions, e.g. crystallization, order-disorder, structural, ferromagnetic, ferroelectric, having different physical interpretations therein. Parameters of the phenomenological Hamiltonian can be obtained from the *ab initio* calculations or interatomistic computer modeling.

Previous attempts to describe heat release along with phase transitions had been based on heuristic ideas; my objective was to develop *a thermodynamically consistent* approach [23]. The free-boundary problem is just a limiting case of this theory when the thermal length and the radius of curvature of an interface are much greater than its thickness. The analysis of systems with slow heat conduction shows that an adiabatic transition is possible such that the temperature of the final phase *is higher than the equilibrium temperature* (metastable or superheated phase production) [5, 6, 8, 10, 12, 15, 17, 21, 23]. This effect was called "heat-trapping" by analogy with the solute-trapping or partitionless solidification of alloys.

Close to the critical point the first-order transitions exhibit intriguing examples of *periodic pattern formation* when the transformation takes the path analogous to the spinodal decomposition characterized by the conserved order parameter (composition) although the original parameter is non-conserved (e.g. magnetization). This means that a weakly first-order transition can proceed by a *continuous modulation mechanism* controlled by heat-transfer [5, 15, 17, 18, 19]. For the case of a structural transition where the order parameter is strain, we demonstrated that estimated properties of Fe-Pd alloys make this system a possible candidate for such behavior. In simulation of the dynamic behavior of such systems, coarsening of the internal domain structure has been observed to occur on late stages of evolution. In contrast to the well known Lifshitz-Slyozov-Wagner type of coarsening kinetics, valid for a small volume fraction of precipitate, this system, which had the volume fraction of the product phase about 50%, demonstrated absolutely different type of the second-phase coarsening behavior, whose distinguished feature was period doubling [17].

A thermal effect has been predicted in materials that underwent a second-order (continuous) transition, e.g. ferromagnetic, or order-disorder, despite the lack of the latent heat in transitions [5, 8, 13]. For instance, in materials with small thermal conductivity motion of the domain walls will proceed much slower than according to the predictions of the Landau-Lifshitz or Cahn-Allen theories that does not take the energy effect into account. This effect may be important for the theory of the hysteresis loop and magnetization dynamics and the continuous transition itself, changing time exponents of the latter.

Change of the crystalline symmetry is usually accompanied by the development of the misfit strain in materials as a result of different lattice spacings in different phases. Small precipitates grow usually without loss of coherency on their interfaces. In my next project I have developed a consistent continuum approach to the problem of segregation at coherent interfaces and incorporated the coherency strain into the continuum model of microstructural evolution of multicomponent alloys [9, 11].

Diffusion and coarsening in multicomponent alloys. [Ref. 16]

The widespread use of multicomponent alloys for the first-principals designing of new smart materials has stimulated my interest in *coarsening process in multicomponent systems* whose thermodynamics is different from that of binaries due to presence of many different components. It was necessary to analyze this process without simplifying assumptions on the solution thermodynamics of alloys that are usually not confirmed in practice. The derived coarsening behavior showed marked departure from a binary case and turned out to be a fundamental contribution to an interdisciplinary program of applying physics, mechanics and materials science to alloy design [16]. This work was tested with the experimental results on the small angle neutron scattering in model alloys and at present is used in the conceptual designing of practical alloys.

Nanomaterials. [Ref. 14, 17]

Nanotechnology is defined as the creation of functional materials, devices and systems with at least one characteristic dimension at the scale of one to one hundred nanometers. It requires fundamental understanding of self-organization at the nanoscale. My interest in nanotechnology and organization at the nanoscale arose from the thermodynamic analysis of *small adiabatically insulated particles*. It showed that their phase diagrams are more complicated than those of large ones: phase separation does not occur when it is supposed to. Instead, there is a considerable extension of the single-phase regions of ordered and disordered phases into the two-phase zone of the phase diagram. Moreover, in a particular energy band, equilibrium is achieved on the homogeneous transition state that corresponds to the saddle point of the free energy [14]. Mechanical, electromagnetic and optical properties of such a state are different form those of the bulk phases. Such particles provide opportunity to study the intrinsically unstable segments of the free energy of materials. This work has also very important ramifications on the theory of amorphization of pure metals.

Many microelectronics devices rely on nanometer-scale films of solid solutions grown on substrates by different deposition techniques. Such films have properties very different from their bulk counterparts. For instance, silicon based semiconductors possess wider than normal band gaps, SnGeTe thin films become superconducting and gain anomalous Hall effect when alloyed with In. Semiconductor films may be grown in such a regime that the band-gap can be tuned by simply changing the dimensions of the material. Fe-Cu and Fe-Ag binary systems are virtually immiscible in the bulk. However, 70 nm nanoparticles of these materials were found to form supersaturated solid solutions. This inspired me to use the mean-field method in order to study the phase transitions in nanofilms of solid solutions [Grant].

BIOPHYSICS

Biophysics of neurons. [Ref. 1]

Acetylcholinesterase (AChE) is an enzyme, which is classically known for its role in hydrolyzing neurotransmitters that diffuse across the synaptic cleft in the process of neuron-muscle cell communication. Recent studies, however, suggest that AChE may have a broader role, particularly in the development of nervous system. Deviations in normal levels of AChE at the initial moments of nervous system development appear to contribute to observed neuro-anatomic abnormalities such as altered neurite (axons and dendrites) outgrowth. Sequence similarities of AChE to some cell adhesion molecules appear to indicate its structural role of neurite adhesive in neuron development process. In this study, we used physical methods to explore the influence of different AChE inhibitors on the normal outgrowth of neurites of the specific neuroblastoma cells. Our results support the hypothesis that AChE promotes neurite outgrowth through adhesive function.

Origin of life research. [Ref. 2, 7]

The experimental findings of the last couple of years inspired my interest in biophysical problems of the origin of life. Almost all tenable hypotheses of the origin of life on Earth describe transformation from geochemistry to biochemistry, which brought about the material of life, DNA-protein combination, and cellular organization of that material. Living organisms, however, are distinguished from a mixture of organic molecules by their high level of complexity, which allows them to carry out certain functions. I analyzed the hypothesis that the earliest forms of life (protocells) were formed through the process of phase transitions, e.g. crystallization. According to this hypothesis, inorganic materials helped build living systems by lending them functions so that organic chemical evolution is just one natural consequence of the evolution of matter in the universe. A self-replicating biological system with adaptation emerged from single molecules using completely abiotic mechanism of formation. This mechanism acted simultaneously at different places on the early Earth and created similar materials everywhere. Hence, the similarities in the living systems did not appear by chance, but as a necessity.

Synergetic approach in medicine. [Ref. 4]

Conventional wisdom in physiology and medicine (theory of homeostasis) holds that a healthy organism regulates itself to maintain constant rhythm, while erratic behavior of the organism is symptomatic of unfolding disease because it suppresses natural rhythms. However, interdisciplinary discoveries of the past decade in mathematics and human physiology convinced many practitioners that chaos in bodily functioning is not necessarily a bad thing. We have qualitatively analyzed many different cases of pathological symptoms in biological systems that may be explained as manifestation of the chaotic behavior and revealed the adaptive nature of chaos in them. The benefit of chaos in physiological systems is stability of the organism, structural or functional, as opposed to instability or death. A new, seemingly universal feature of the dynamical systems controlled by a chaotic subsystem was revealed. To delineate this feature we proposed the principle of compensation, according to which the loss of controlling function of one subsystem of a defective system may be compensated by chaotic behavior of another subsystem, less important for "survival" of the whole system. Briefly speaking, we are wired such that if a central organ fails, a peripheral one comes to rescue. Application of this principle to medicine may bring new treatment strategies.

LIST OF THE MOST IMPORTANT PUBLICATIONS

Overall I have published over 40 articles and papers on different subjects of condensed-, soft-matter, computational materials physics, and biophysics. Many of the publications are available on my website. (*) means an undergraduate student.

1. "Structural Impact of Diazinon and Molinate on Neurite Outgrowth in N1E-115 Cells" D.T. Edge (*), R.D. Cannady (*), J.S. Ross (*), A. Umantsev, and S.L. Chao. J. Neurosci. Res. In preparation.
2. "On the structure and formation of a protobiont", A. Umantsev. Origins of Life and Evolution of the Biosphere. Submitted.
3. "Early stages of soldering reactions", R.A. Lord (*) and A. Umantsev. Acta Mater. Submitted.
4. "Adaptive Chaos: Mild disorder may help contain big disease" A. Z. Golbin and A. Umantsev, Journal of Theoretical Medicine. Submitted.
5. "Thermal effects in phase transformations: A review", A. Umantsev. Journal of Elasticity. Accepted.
6. "Physical analogy between continuum thermodynamics and classical mechanics", A. Umantsev. Phys. Rev. E **69**, 016111 (2004).
7. "Exploring the structure of a hydrogen cyanide polymer by electron spin resonance and scanning force microscopy", M.P. Eastman, F.S.E. Helfrich (*), T.L. Porter, A. Umantsev and R. Weber. Scanning. **25**(1), 19-24 (2003).
8. "Thermal effects in dynamics of interfaces", A. Umantsev. J. Chem. Phys. **116** (10), 4252-4265 (2002).
9. "Coherency strain assisted equilibrium segregation at heterophase interfaces", A. Umantsev. Interface Science, **9** 237-242 (2001).
10. "Thermal effects of interfacial dynamics", A. Umantsev. Interface Science, **9** 349-356 (2001).
11. "Continuum theory of interfacial segregation", A. Umantsev. Phys. Rev. B **64** p.075419-075429 (2001).
12. "Thermal effects of interface motion". In *Interfaces for the 21st Century: New research directions in Fluid Mechanics and Materials*, (Imperial College Press, 2002) p. 286. *Proceedings of the Conference*: "Interfaces for the Twenty-First Century", Monterey, California, 15-18 August (1999)

13. “Thermal drag of the antiphase domain boundary motion”, A. Umantsev. Acta Mater., **46** (14), pp.4935-4939, (1998).
14. “Adiabatic phase transformations in confinement”, A. Umantsev. J. Chem. Phys. **107**(5), pp1600-1616, (1997).
15. “Continuum methods in the kinetic theory of phase transformations”. *Proceedings of the PTM'94*, Pittsburgh, PA, July 17-22, p.31, (1994).
16. “Ostwald ripening in multicomponent alloys”, A. Umantsev & G.B. Olson. Scripta Metal et Material, **29** 1135-1140, (1993).
17. “Phase equilibria and transformations in adiabatic systems”, A. Umantsev and G.B. Olson. Phys.Rev. E **48** (6), 4229-4249, (1993).
18. “Modulation mechanism for displasive transformation”, A. Umantsev and G.B. Olson. *Proceedings of the ICOMAT'92*, Monterey Institute of Advanced Studies, Carmel CA, 20-24 July, p.215 (1992).
19. “Modulation mechanism for first-order transformations with nonconserved order parameter”, A.Umantsev & G.B. Olson. Phys. Rev.A **46** (10), Rapid Communications R6132-R6135, (1992).
20. “Growth from a hypercooled melt near absolute stability”, A. Umantsev & S.H. Davis. Phys.Rev. A **45** (10), 7195-7201, (1992).
21. “Thermodynamic stability of phases and transition kinetics under adiabatic conditions”. A.Umantsev. J. Chem. Phys. **96**(1), 605-617, (1992).
22. “Microstructure formation of the melt-spun crystalline ferrous ribbons”. *Institutional report*, National Research Laboratory for Metallurgy, 1989
23. “Nonisothermal relaxation in a nonlocal medium”, A. Umantsev and A. Roytburd. Sov. Phys. Solid State **30**(4), 651-655, (1988).
24. “Physical and chemical methods increasing homogeneity of metal during casting”. *Institutional report*, National Research Laboratory for Metallurgy, 1988.
25. “Simulating dendritic structure-formation in the crystallization of a supercooled liquid, A. Umantsev, V.Vinogradov & V.Borisov, Industrial Laboratory, **52** (7) 1987, pp. 638-641.
26. “Theoretical development of thermophysical aspects of control algorithm of the thermal regime of solidification”. *Institutional report*, National Research Laboratory for Metallurgy, 1987.

27. “Modeling the evolution of a dendritic structure”, A. Umantsev, V.Vinogradov and V.Borisov. Sov. Phys. Crystallography **31** (5), 596-599, (1986).
28. “Computer simulation of a dendritic structure formation during solidification of metals and alloys”. Abstract of Ph. D. Thesis, 1985.
29. “Numerical simulation of dendritic structure”. *Proceedings of All Union Conference on Crystal Growth.* Tzahkadzor, Armenia, September 1985
30. “Mathematical model of growth of dendrites in a supercooled melt”, A. Umantsev, V.Vinogradov and V.Borisov. Sov. Phys. Crystallography **30** (3), 262-265, (1985).
31. “Motion of a plane front during crystallization”, A. Umantsev. Sov. Phys. Crystallography **30** (1), 87-91, (1985).

OUTLINE OF MY TEACHING PHILOSOPHY

Teaching is a value-laden activity. I find teaching to be rewarding on many levels, including student mentoring, lecturing, recitation, and curriculum planning. My objectives as a teacher are to achieve excellence in undergraduate education and to convey the excitement of sciences to general students. I hope to foster critical thinking, facilitate the acquisition of life-long learning skills, and develop problem-solving strategies. I also want to make a difference in the lives of my students and prepare them for wider range of career opportunities in an information economy. To function effectively in small companies the graduates will be expected to combine many different skills: fundamental knowledge, hands-on experience, computational experience, and teamwork.

In my lectures I require students to understand the fundamental concepts underlying the material. Above all, however, I am interested in mechanisms that help students come to appreciate the beauty and wonder of Physics. Scientists discover new things by doing experiments, making observations, and immersing themselves in the subject. If we hope to inspire students to become scientists or even expect them to respect what scientists do, we have to find a way to show them the excitement of discovering something new, of experiencing the acquisition of new scientific knowledge. I aspire to challenge students to truly engage with the subject matter and give them firsthand experience with the magnificence of science.

Traditional physics courses and classroom problem solutions do not always help our students to see "how objects move in space and time". As an educator I am trying to broader utilize in my classroom national-level teaching methods and contemporary interactive educational technology in the form of computer simulations and web-based physics courses. This improves an effective, active-learning environment and does not compromise intellectual standards.

I value process of critical thinking, independence, and individual problem-solving skills. To verify if this objective has been reached, I develop my exams to test students' ability to solve problems. I also value group skills and cooperation. In order to develop these skills I use hands-on laboratory experience and help students attain the highest level of performance that I am seeking. I have developed my own evaluation means that are more directly related to the specific goals and objectives that I am trying to achieve in education. In this evaluation questionnaire I am asking the students to reflect on the most important aspects of the lecture and hands-on courses.

In the future I intend to:

1. Develop an interdisciplinary unifying curriculum for Science Education, which includes Mathematics and Chemistry courses together with regular courses in Physics. Implementation of such curriculum requires cooperation with other departments' members.
2. Develop an Astrobiology Program (in cooperation with Biology Departments' members).
3. Develop or strengthen an already existing Biophysics program.
4. Develop a Computational Biophysics course, which will give the student a firm basis in the main computational techniques used in modern physics.
5. Communicate the role, importance, and impact of physics, engineering and astronomy to the community. Work with high school science teachers to promote the pre-college Science Education, getting young people interested in different areas of physics.

Computational Biophysics

Outline of the proposed course

The use of computers in physics and other branches of science and engineering has increased tremendously along with rapid development of faster and cheaper hardware. This course will aim to give the student a thorough grounding in the main computational techniques used in modern physics and biophysics. It will be particularly important in the course that the students will be learning by doing. The course is therefore designed in such a way that a significant fraction of the students' time is spent actually programming for specific physical problems rather than learning abstract techniques. This is, however, neither a short course in computing science, nor in programming. It focuses specifically on methods for solving physics problems. The students will be expected to be familiar with basic programming techniques.

The course will cover broad sections:

- Interpolation and extrapolation.
- Numerical methods for ordinary differential equations.
- Linear systems.
- Numerical methods for partial differential equations.
- Monte Carlo and other simulation methods, such as molecular dynamics.
- Scientific visualization.

Project material may come not only from physics, but also from mathematics, chemistry, biology, and medicine. It will focus on realistic physical problems, which apply and extend the techniques:

- Chaos from non-linear dynamical systems and mappings.
- Phase transitions and magnetization (Ising model).
- Monte Carlo methods for surface particle transport.
- Crystal growth and diffusion limited aggregation (DLA).
- Seismic wave propagation and ocean circulation models.
- Biophysical problems.
- Computer simulation of evolutionary and population genetics processes.
- Cardiac dynamics.
- Issues in computational astrophysics.

Text and reference books:

1. H. Gould and J. Tobochnick "An Introduction to Computer Simulation Methods", Addison-Wesley.
2. N.Gershenfeld "The Nature of Mathematical Modeling", Cambridge.
3. W. Press, B. Flannery, S. Teukolsky, W. Vetterling "Numerical Recipes" Cambridge.
4. Caswell, H. 1989. Matrix Population Models. Sinauer Associates, Sunderland.

Life in Cosmos

The course will be open to all students; no prior knowledge of astronomy, physics or biology will be assumed or required.

Because new planets are being created and discovered all the time, scientists believe there may be as many as 10 billion earth-like planets in the universe. Thus the odds of primitive life existing elsewhere in the cosmos are very high. Many of modern scientists believe that extra-terrestrials not only exist, but may be sending us signals at this very moment. Others think that there may be many examples of primitive life to be found in the Cosmos, advanced intelligent life (like ours), however, may be very rare.

The aim of this course is to convey the detailed conceptual ideas associated with the important and topical question of the formation of life in the universe. The course will discuss all the environmental circumstances that seem to encourage the start of any life form and investigate the current state of our knowledge of life outside of the earth. These questions are looked at from a multi-disciplinary viewpoint, which includes astronomy, biology, chemistry and geology. However, other issues such as the historical, cultural and philosophical perspectives are included.

This course addresses the fundamental questions:

- Are we alone?
- What are the prospects for intelligent life elsewhere in the Universe?
- How do we search for evidence of such life?
- Will life only be found in the traditional "comfort zones" of solar systems?
- Where are complex hydrocarbons and other sophisticated molecules found in space?
- How are they created, and how do they survive?

The major topics of the course are:

- The evolution of life on Earth, including examples of life that don't appear to require sunlight and/or oxygen to survive.
- The evidence for possible astronomical causes of major mass extinctions.
- The possible origin and evolution of life in an extraterrestrial planetary context: the birth of exobiology.
- A discussion of the panspermia theory for the spreading of life through the solar system.
- Life in the Solar System: our expectations about potential life on Mars, Europa and elsewhere.
- Searching for other planetary systems: a detailed discussion of the techniques used, and the recent discoveries of the many planetary systems around nearby stars.
- The astronomical background to the Drake Equation, in particular, the evolution of stars and planetary systems.
- SETI: searching for signals from extraterrestrials and the intrinsic difficulties in communicating with, and visiting, other “civilizations”.

Text and reference books:

1. “An Introduction to Astrobiology” Edited by Ian Gilmour and Mark A Sephton, (Cambridge University Press, Open University Textbooks, 2004).
2. Zubay, G., “Origins of Life on the Earth and in the Cosmos” (Academic Press, N.Y. 2000)
3. “Life in the Universe”, Jeffrey Bennett, Seth Shostak, and Bruce Jakosky, (Addison Wesley).