10 Project Proposals in Material Science from Igor Sikorsky Kyiv Polytechnic Institute

1. Project Proposal Information

Project Proposal Title	Formation of nanodimensional film of Co, Mn, Ni, Ti, Ta, Pt transition metal silicides on monocrystalline silicon with controlling thermal stability and resistivity using diffusion-controlling membranes
Keywords	nanodimensional silicide films
Abstract (Max. 2000 words)	The project aims is to establish the regularities of formation of nanoscale films silicides of Co, Mn, Ni, Ti, Ta, Pt thermally stable in the range 400-1000°C on single-crystal silicon Si (001).
Project Description (Main Work Packages)	It is planning to investigate the conditions of diffusion formation of thermally stable nanoscale monosilicide Ni films. It is proposed to solve this by doping the nickel film during the co-deposition of nickel and platinum, or by the use of additional layers as diffusion barriers and sources of alloying elements to optimize nickel and silicon interdiffusion rate during annealing. As regulators of the diffusion processes Ti, C, Pt etc. layers will be used.

Project Proposer Information

Name of the Organisation	National Technical University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute”
Organisation Type	Research University
Country	Ukraine
Fields of Activity	Formation of nanodimensional film of Co, Mn, Ni, Ti, Ta, Pt transition metal silicides on monocrystalline silicon with controlling thermal stability and resistivity using diffusion-controlling membranes Improvement of magnetic properties of nanodimensional films for ultrahigh density magnetic recording and information storage Formatıon of phase composıtıon and structure ın nanodımensıonal fılms on base of $CoSb_3$ skutterudıte – functıonal elements of thermoelectrıcity

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2. Project Proposal Information

Project Proposal Title	Formation of phase composition and structure in nanodimensional films on base of $CoSb_3$ skutterudite – functional elements of thermoelectricity
Keywords	nanodimensional thermoelectric films
Abstract (Max. 2000 words)	Thermoelectrics is priority direction of development of science and technique based on the direct conversion of thermal energy into electric. Absence of moving parts and possibility of functioning in extreme conditions provide a high reliability and practically unlimited resource of work to the thermoelectric energy sources. The special advantage is using the thermal energy that is lost. For this reason such sources are founded wide application in space, in a military technique and in the way of life.
Project Description (Main Work Packages)	The conversion efficiency is determined by dimensionless figure of merit $$ZT=S^2 \sigma T/(k_e+ k_l),$$ where σ is thermal conductivity, S is Seebeck coefficient, T is temperature, k_e is the carrier thermal conductivity, k_l is the lattice thermal conductivity). In spite of active attempts to get material with the high value of ZT nowaday thermoelectric elements which in majorities are synthesized by the methods of powder metallurgy have ZT which does not exceed 1. In the

	nanodimensional film state ***ZT,*** as theoretical calculations show, can have value ≥ 2. It is explained that at transition to nanodimensions the electron-phonon interaction decreases and a phonon subsystem, being adiabatically isolated, does not almost accept participating in the transfer of heat from a heater to the cooler. Therefore nanostructuring of thermoelectric materials is effective technology to achieve a high ***ZT*** due to achievement of low thermal conductivity. It is suggested to use the nanodimensional $CoSb_3$ –based skutterudite film as thermoelectric material with high-performance thermoelectric properties. A lattice thermal conductivity can be considerably reduced due to decrease of size of grains that results in additional scattering of phonons on the grain boundaries, and also presence of pores in films. One of the special properties of skutterudite compounds there is also possibility of decrease of lattice thermal conductivity when small in size atoms fill pores in the crystalline structure of skutterudite. Alloying atoms (filler of pores), for example, the atoms of elements of Ba, Yb, Tl, Ce, La, at resonance frequency additionally scatter heat, what is carried by phonons, that results in the lower thermal conductivity of film. Due to it thermoelectric efficiency of ***ZT*** can attain the value more than 1,4. Nanodimensional $CoSb_3/SiO_2$(100 nm)/Si(001) film compositions of nanometer (10 – 50 nm) thickness will be obtained by co-deposition of Co and Sb in vacuum of 10^{-9} Pa on substrates of monocrystalline Si(001) covered SiO_2 layer at room temperature or heated to temperature in the range (370 – 570)K. Sb deposition will be carried out by effuser and Co – by electron-beam methods. For alloying of film it will be used Ba, Yb, Tl, Ce, La. For thermal treatment it will be applied annealing in nitrogen or vacuum in temperature range of (570 - 970)K.

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Organisation Type	Research University
Country	Ukraine
Fields of Activity	Formation of phase composition and structure in nanodimensional films on base of $CoSb_3$ skutterudite – functional elements of thermoelectricity Formation of nanodimensional film of Co, Mn, Ni, Ti, Ta, Pt transition metal silicides on monocrystalline silicon with controlling thermal stability and resistivity using diffusion-controlling membranes Improvement of magnetic properties of nanodimensional films for ultrahigh density magnetic recording and information storage
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3. Project Proposal Information

Project Proposal Title	Improvement of magnetic properties of nanodimensional films for ultrahigh density magnetic recording and information storage
Keywords	nanodimensional magnetic films
Abstract (Max. 2000 words)	Creation of devices with ultrahigh-density magnetic recording and storage of information is a significant problem of the modern science and technique. The increase of recording density by traditional methods already attained a limit. Now for the storage of digital

	information the magnetic disks are applicated, for the fabrication of which the layer of magnetic material is deposited on the unmagnetic substrate and then a recording is carried out. As magnetic material (a magnetic recording media) it is applicated both polymeric coverage, which contains magnetic one-domain particles (as a rule y-Fe_2O_3), and thin (of (50 – 150) thick nm) film of magnetic metal, alloy or oxide (alloys are usually utilized on the basis of Co, for example, Co-Ni, Co-Ni-W, Co-Pt-Ni et cetera). Size of magnetic domains located in a few grains is ~ 100 nm. Thin magnetic films have a grain structure with the size of grain of film thickness. Coercivity of magnetic materials which are used for the storage of information lies in a range from 8 A/m to 37 A/m, and remanence arrives for 1,5 T. Reached density of magnetic recording and storage of information is 10-15 Gbit/cm^2. For the subsequent increase of density the new nanodimensional materials with lower-limit dimension of magnetic domains located in isolated grain with size of 5-15 nm are needed, which allow to fabricate recording medium of new generation with ultrahigh-density magnetic recording and storage of information (to 1 Tbit/cm^2). For creation of such magnetic writing devices the magnetic ordered $L1_o$-FePt phase with face-centered tetragonal structure can be used due to its large uniaxial magnetocrystalline anisotropy energy ($7 \cdot 10^6$ J/m^3 that more than on an order higher than in the magnetic recording medium, which are used) to high chemical and to anticorrosive stability. The methods of fabrication and thermal stabilization of nanodimensional (10 -30 nm) magnetic ordered $L1_o$-FePt films, management an orientation of the easy magnetization axis and magnitude of coercivity are developed. Decrease the temperature of the magnetic ordering and increase thermal stability of magnetic of $L1_o$-FeP films with the size of grains to (5 – 15) nm can be carried out due to introduction of interface energy by the use of additional layers of Cr (Au, Ag) or combinations of Pt/Cr (or Pt/Ag) in film composition of FePt/additional layer/substrate or multi-layered film

	composition of Fe/Pt/Fe/Pt/…, what will provide a driving force for ordering of FePt film using tension energy between FePt film and additional layer for acceleration of the ordering process. Also it is assumed that diffusion the third element with low surface energy such as Co (or Au, Ag, Sb, Bi) will stimulate the rearrangement of Fe and Pt atoms and will ensure the ordering process. Alloying atoms located on the boundaries of FePt grains carry out control for the size of grain and slow motion of domain wall of FePt during the demagnetization process that favour the increase of coercivity.
Project Description (Main Work Packages)	For formation of the controlled orientation of grains - textures in $L1_o$-FePt films it will be used the different substrates such as SiO_2/Si(001), amorphous particles of SiO_2 of spherical form, glass, polystyrene both at a room temperature and heated to the temperatures in the range of (620 - 770) K. At application of amorphous substrates it is assumed the using the seed layers in particular Cr(100), MgO(100). Fabrication of nanodimensional film in thick of 10- 30 nm on the basis of magnetic ordered $L1_o$-FePt phase by the method of magnetron sputtering with the use of the mosaic targets from the metals of Fe and Pt with the alloying elements of C, Ag, Ni, B, Cu, Au, Sb on substrate of SiO_2 or MgO, CrRu, CrMo. Heat treatment carries out by method of the thermal annealing in nitrogen or vacuum in the temperature range of (620 – 970 K) with different rates of heating and duration. For the magnetic recording of information by $L1_o$-FePt film it is possible to use technology of the thermally activated magnetic record (TAMR) at cooling from the paramagnetic state.

Project Proposer Information

Name of the Organisation	National Technical University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute”
Organisation Type	Research University
Country	Ukraine
Fields of Activity	Improvement of magnetic properties of nanodimensional films for ultrahigh density magnetic recording and information storage

	Formation of nanodimensional film of Co, Mn, Ni, Ti, Ta, Pt transition metal silicides on monocrystalline silicon with controlling thermal stability and resistivity using diffusion-controlling membranes Formatıon of phase composıtıon and structure ın nanodımensıonal fılms on base of $CoSb_3$ skutterudıte – functıonal elements of thermoelectrıcıty
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4. Project Proposal Information

Project Proposal Title	Formation of biocompatible hydroxyapatite composite coating reinforced with carbon nanotubes on titanium alloys
Keywords	Biocompatible materials, titanium alloys, coatings, high-energy treatment methods
Abstract (Max. 2000 words)	Forming scientific basis for the development of technology of composite biocompatible coatings on titanium alloys used in prosthodontics and implants, based on the effect of the interaction of carbon nanotubes with hydroxyapatite treated with a high-laser radiation, to improve the physical and mechanical properties (adhesion, long-term stability etc.) and extending the use of implants and prostheses in the body rights.
Project Description (Main Work Packages)	Therefore, development of technologies for biocompatible coatings with high adhesion and a wide set of service characteristics is the actual task facing researchers at the intersection of materials science and medicine. Main Work Packages: testing method of forming nanotubes and determine optimal parameters of processes, a carbon nanotubes and studied their

	structure, study processes that occur in chemically inert substrates in vacuum at high-temperature annealing of thin films of metal-catalysts; establishing patterns of flow processes on the interfaces: carbon nanotube - hydroxyapatite and structural study of phase transformations on it, develop a working hypothesis processes of interaction of laser ablation of hydroxyapatite with carbon nanotubes in vacuum at different temperatures, density, power deposition process of composite coatings, based on established patterns to develop theoretical foundations and laboratory technology for biocompatible composite coatings, analysis and synthesis of research, establishing patterns and mechanisms of formation of the biocompatible composite coatings.

Project Proposer Information

Name of the Organisation	National Technical University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute”
Organisation Type	Research University
Country	Ukraine
Fields of Activity	Formation of biocompatible hydroxyapatite composite coating reinforced with carbon nanotubes on titanium alloys Biocompatible materials, titanium alloys, coatings, high-energy treatment methods
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5. Project Proposal Information

Project Proposal Title	High temperature X-ray analysis of nanocrystalline magnetically soft iron alloys and optimization their properties after stage-by-stage heat treatment
Keywords	Nanocrystalline magnetically soft materials, iron alloys, coatings
Abstract (Max. 2000 words)	Establish the optimal parameters of heat treatment of nanocrystalline soft magnetic iron alloys to achieve high magnetic properties through analysis of structural and phase state using high-temperature X-ray
Project Description (Main Work Packages)	Nanocrystalline soft magnetic materials with properties superior to traditional crystalline materials. Such magnetic properties as coercively, magnetic permeability and magnetization largely depend on the structural state and phase composition of the alloy after heat treatment. Therefore, to achieve optimum properties of these materials to research the process of structural and phase transformations during heat treatment. We also need to develop new modes of non-isothermal heat treatment, which would be due to changes in the duration and temperature at certain stages of the process led to the formation of structural and phase components that will ensure minimum coercive field and maximum values of permeability and magnetization that can be applied to this alloy.

Project Proposer Information

Name of the Organisation	National Technical University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute”
Organisation Type	Research University
Country	Ukraine
Fields of Activity	High temperature X-ray analysis of nanocrystalline magnetically soft iron alloys and optimization their properties after stage-by-stage heat treatment Coatings, high-energy treatment methods, X-ray analysis
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6. Project Proposal Information

Project Proposal Title	Formation of carbon-hardening and nitrogen containing subsurface of iron alloys by electro-spark and laser alloying methods
Keywords	Subsurface, iron alloys, coatings, electro-spark alloying, laser treatment, phase structure
Abstract (Max. 2000 words)	The project envisaged to establish the physical basis of forming coatings containing carbides and nitride phases processes formed by the interaction of elements saturation environment (nitrogen and carbon) of metals incorporated in alloys of iron and transition metal alloying by electrode (zirconium, titanium, chromium). Creating carbide-nitride coating on the surface of iron alloys occur under intense processes of high-energy treatment – electro-spark alloying (ESA) and laser alloying (LA).
Project Description (Main Work Packages)	It is expected that obtained by electro-spark and laser alloying treatment coatings will have superfine carbide, nitride and carbide-nitride phases. This is provide new physical and mechanical properties, in particular, higher hardness and wear resistance compared to the hardness and wear resistance obtained with traditional chemical-heat treatment. To establish patterns of these type coatings will focus on structural and phase transformations occurring during ESA and LA, the influence of saturation environment on the structure and properties of the alloy subsurface and defined its optimal composition.

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Organisation Type	Research University
Country	Ukraine
Fields of Activity	Formation of carbon-hardening and nitrogen containing subsurfaces of iron alloys by electro-spark and laser alloying methods Coatings, high-energy treatment methods, X-ray analysis
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7. Project Proposal Information

Project Proposal Title	The creation of surface nano-structural layers on products working at extreme loading conditions by methods of high energy influence and frictional treatment
Keywords	Materials that allow operation at high temperature, materials' in-service properties, corrosion resistance, erosion resistance, radiation resistance, reliability and durability, ionic conductivity and mechanical properties
Abstract (Max. 2000 words)	The project is aimed on the development of a new conceptual resource-saving technology for surface modification and recovery of machine components working at extreme conditions by creation of nanostructures coherently bounded to each other that will support the high level of service properties which cannot be achieved using the most advanced construction materials and will increase 2-3 times components service life

Project Description (Main Work Packages)	A system of measures is suggested in the project which will permit to improve significantly both the mechanical properties of the structures and to increase their resistance to service loads and action of such media which cause their premature failure, namely: - new ecologically clean technologies of deposition of filler materials and their remelting in vacuum to produce nanostructures and to increase the strength of their adhesion with a base metal; - new combined mixtures of powder materials will be used to impart the new properties to the surfaces being treated; - new principle of improving the properties of surface layers at high unit loads will be developed by deposition of multilayer coatings where the upper layers will bear the main loads and the intermediate layers will be damping, i.e. they will suppress and distribute the peak loads; - new data will be obtained concerning characteristics of nanostructures of the surface layers under the conditions of the highest loads or action of special media. The obtained results will give an opportunity to develop the bimetal coatings to use them in food, chemical and gas industries, in the development of electrical contacts, in the aircraft industry for the treatment and restoration of the surface of blades or other components of gas turbine engines, etc. The application of original coating mixtures and combined high energy treatment technique will allow to obtain the coatings with a preassigned type of concentration and phase distributions on the hot-strength Ni and Cr – base alloys with controlled regulation of structure from nano- to microsize scale, without surface and inner defects. The increasing alloying elements content in studied alloys in comparison with traditional steels provide high-temperature strength growth up to 1300 K and

	technological properties enhancement. Development of scientific principles for creation of surface nano-structured layers supporting a high level of service properties on the products working at extreme loading conditions will allow enhance twice mechanical properties of the coating and substantially increase tribological and service properties that according to world level of theoretical and applied researches in this scientific direction.

Project Proposer Information

Name of the Organisation	National Technical University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute”
Organisation Type	Research University
Country	Ukraine
Fields of Activity	The creation of surface nano-structural layers on products working at extreme loading conditions by methods of high energy influence and frictional treatment Controlled regulation of structure and phase formation processes in Ni and Cr - base multicomponent systems by high energy sources Formation and investigation of the solid coatings from aluminides with high hardness and fracture toughness characteristics
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8. Project Proposal Information

Project Proposal Title	Formation and investigation of the solid coatings from aluminides with high hardness and fracture toughness characteristics
Keywords	Materials that allow operation at high temperature, materials' in-service properties, corrosion resistance, erosion resistance, radiation resistance, reliability and durability, ionic conductivity and mechanical properties
Abstract (Max. 2000 words)	The creation of wear resistance hard coatings with high fracture toughness on aluminium-based alloys is one of the main problems of searching of many scientists from the well-known firms worldwide, the solution of which would allow to increase the components lifetime of aircraft and automobile machines. The attention is paid to the creation of the alloys with nano- and quasicrystalline structures under the particular conditions and that could be used for the strengthening of wear resistive coatings for the parts of mechanical engineering. One of the methods is the obtaining of the quasicrystalline coatings from the aluminides. .
Project Description (Main Work Packages)	The enhancement of tribotechnical properties of modern aluminium-based alloys by coating of the working surface of components is so important. The purpose of this investigation is creation of the aluminides coatings by using ion-plasma technology deposition which due to the untraditional atomic structure and developed intermediate layer has improved physical and mechanical properties

Project Proposer Information

Name of the Organisation	National Technical University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute”
Organisation Type	Research University
Country	Ukraine
Fields of Activity	The creation of surface nano-structural layers on products working at extreme loading conditions by methods of high energy influence and frictional treatment

	Controlled regulation of structure and phase formation processes in Ni and Cr - base multicomponent systems by high energy sources Formation and investigation of the solid coatings from aluminides with high hardness and fracture toughness characteristics
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9. Project Proposal Information

Project Proposal Title	Controlled regulation of structure and phase formation processes in Ni and Cr - base multicomponent systems by high energy sources
Keywords	Materials that allow operation at high temperature, materials' in-service properties, corrosion resistance, erosion resistance, radiation resistance, reliability and durability, ionic conductivity and mechanical properties
Abstract (Max. 2000 words)	The purpose is the creation of principals for the surface layers structure control of hot-strength Ni and Cr – base alloys and development on these data of new conceptual resource-saving technology for the surface modification and repair of components and machine parts working in extreme conditions to support high level of service properties which could not be achieved even using of the latest solid construction materials. The application of original coating mixtures and combined high energy treatment technique allows to obtain the coatings with a preassigned type of concentration and phase distributions on the hot-strength Ni and Cr – base alloys with controlled regulation of structure from nano- to microsize scale,

	without surface and inner defects. The increasing alloying elements content in studied alloys in comparison with traditional steels provide high-temperature strength growth up to 1300 K and technological properties enhancement..
Project Description (Main Work Packages)	The application of original coating mixtures and combined high energy treatment technique allows to obtain the coatings with a preassigned type of concentration and phase distributions on the hot-strength Ni and Cr – base alloys with controlled regulation of structure from nano- to microsize scale, without surface and inner defects. The increasing alloying elements content in studied alloys in comparison with traditional steels provide high-temperature strength growth up to 1300 K and technological properties enhancement.

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Organisation Type	Research University
Country	Ukraine
Fields of Activity	The creation of surface nano-structural layers on products working at extreme loading conditions by methods of high energy influence and frictional treatment Controlled regulation of structure and phase formation processes in Ni and Cr - base multicomponent systems by high energy sources Formation and investigation of the solid coatings from aluminides with high hardness and fracture toughness characteristics
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10. Project Proposal Information

Project Proposal Title	The influence of processes on the outer surface of thin metal layers on diffusional phase formation in a volume
Keywords	thin metal layers, nanostructure, diffusion, surface
Abstract (Max. 2000 words)	Fundamental studies of the impact processes that take place onto external surface of thin subsurface layers and layered composites of pure metals and alloys with submicron and nanoscale thicknesses (including biocompatible metallic materials and metallic materials for medicine) and govern the development of diffusion controlled formation of phase composition and phase transformations inside inner parts of materials aiming to lay a scientific foundation for basics in advanced technologies for production of nanostructured, nanophase materials and epitaxial layers.
Project Description (Main Work Packages)	This project proposes comprehensive studies of physical and chemical processes on the outer surface of a number of composites (including biocompatible metals and metal medical supplies), the thickness of which can be compared with a length of diffusion path at temperatures of exploitation. Defining the mechanisms and kinetics of diffusion mass transfer at relatively low temperatures to surface layers and processes of phase formation in the volume of compositions that are prospective for practical use, should be considered as relevant scientific challenges. Experimental confirmation of hypotheses and patterns that will be determined, open up new technological possibilities of controlled and pre-designed formation of structure-concentration-phase distribution of substances, allows a new - higher - degree of controllability and repeatability of production processes, layered compositions of metals and metal alloys submicron and nanometer thickness, will allow to achieve a qualitatively new features and performance, will increase yields valid. It will be

	proposed technical solutions in the industry of medical engineering (creating biocompatible coatings on titanium alloys for dentistry, surgery, implantology, prosthetics, etc.) and developed methods for modification of metal surfaces with a view to improving biocompatible implants.

Project Proposer Information

Name of the Organisation	National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"
Organisation Type	Research University
Country	Ukraine
Fields of Activity	thin metal layers, diffusion, nanophase materials
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