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14. ABSTRACT
Mechanical properties of advanced nanostructured ceramic composites are theoretically described with emphasis on the role of defects and interfaces (grain and interphase boundaries) as well as nanoscale effects in these processes occurring at various length scales. In particular, theoretical models are suggested describing (i) emission of partial dislocations from amorphous intergranular boundaries in ceramic nanocomposites; (ii) the role of amorphous intergranular boundaries as toughening elements in nanoceramics; (iii) combined effects of intergrain sliding and diffusion processes on ductility of nanoceramics; (iv) the grain size effect on crack blunting in nanoceramics at elevated temperatures; (v) the strengthening effect of Y-junction nanotubes in ceramic nanocomposites; (vi) nucleation of nanograins near crack tips and its role as a special toughening mechanism in ceramic nanocomposites; (vii) generation of nanoscale cracks at defect configurations formed due to intergrain sliding in nanoceramics.

15. SUBJECT TERMS
Nanostructured materials, nanocomposites, mechanical properties

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Abstract

Mechanical properties of advanced nanostructured ceramic composites are theoretically described with emphasis on the role of defects and interfaces (grain and interphase boundaries) as well as nanoscale effects in these processes occurring at various length scales. In particular, theoretical models are suggested describing (i) emission of partial dislocations from amorphous intergranular boundaries in ceramic nanocomposites; (ii) the role of amorphous intergranular boundaries as toughening elements in nanoceramics; (iii) combined effects of intergrain sliding and diffusion processes on ductility of nanoceramics; (iv) the grain size effect on crack blunting in nanoceramics at elevated temperatures; (v) the strengthening effect of Y-junction nanotubes in ceramic nanocomposites; (vi) nucleation of nanograins near crack tips and its role as a special toughening mechanism in ceramic nanocomposites; (vii) generation of nanoscale cracks at defect configurations formed due to intergrain sliding in nanoceramics.
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Technical Section

Objectives:

(a) Understand and theoretically describe typical defects and interfaces (in particular, non-equilibrium grain and interphase boundaries, amophous intergranular layers) in advanced ceramic nanocomposites fabricated by basic technological routes retaining the nanocrystalline structure.

(b) Understand and theoretically characterize plastic and superplastic deformation mechanisms, including the role of defects and interfaces in plastic flow processes occurring in advanced ceramic nanocomposites at various length scales.

(c) Understand and theoretically characterize mechanisms of nucleation, growth and convergence of cracks/voids in advanced ceramic nanocomposites. Theoretically describe toughening mechanisms, including the effects of defects, interfaces and second phase nanoparticles on nucleation and evolution of cracks as well as suppression of crack initiation and growth in advanced ceramic nanocomposites.

(d) Understand and theoretically describe competition and interaction between plastic deformation and fracture processes occurring in advanced ceramic nanocomposites at various length scales. Theoretically characterize the effects of grain and nanoparticle sizes, nano- and micro-scale inhomogeneities of the structure, strain hardening mechanisms, diffusivity and elastic constants on plastic deformation and fracture processes in these nanocomposites.

(e) Understand and theoretically characterize the effects of fabrication/processing technologies and conditions of mechanical treatment on mechanical properties of advanced ceramic nanocomposites. Predict the interfacial and defect structures, that will optimize and enhance the mechanical properties of these materials.

(f) Understand and theoretically describe the specific transformations of defect structures (first of all, interfacial defect structures), causing enhanced relaxation of residual stresses and stress gradients in nanocrystalline ceramic coatings.

(g) Theoretically reveal new phenomena in advanced ceramic nanocomposites, that can be potentially used in technological applications.

Technical Approach:

In the framework of the research project, exploit methods of conventional and gradient (nanoscopic) elasticity theories of defects and interfaces, geometric theory of grain and interphase boundaries, theories of crack nucleation and growth, with the specific nanoscale effects and the correlation between processes occurring on various length scales taken into account. The focuses were placed on a theoretical description of the role of defects and interfaces in plastic deformation, fracture and toughening mechanisms in ceramic nnocomposites The theoretical models elaborated in the framework of the project used as an input the corresponding experimental data published in the scientific literature (in particular, data of the experimental researches funded by ONR).

Progress (for Research Period from January 01, 2007 until December 31, 2009):

Mechanical properties of advanced nanostructured ceramic composites are theoretically described with emphasis on the role of defects and interfaces (grain and interphase boundaries) as well as nanoscale effects in these processes occurring at various length scales. In particular, a theoretical model is suggested describing emission of partial dislocations from amorphous intergranular boundaries into crystalline grains in deformed ceramic nanocomposites. It is shown that the emission process is energetically favorable in nanoceramics SiC (deformed at high stresses and elevated temperatures) and enhances ductility of these nanoceramics.

Plastic flow in amorphous intergranular boundaries at intermediate temperatures and the role of such boundaries as toughening elements in nanoceramics are theoretically described. It is revealed that plastic flow within intergranular amorphous layers of a-Si3N4 in nanocomposite nc-TiC/a-Si3N4 can initiate cracks.

Also, the combined effects of grain boundary sliding and diffusion processes on ductility of nanoceramics are theoretically described. It is theoretically shown that good ductility of nanocrystalline materials can be reached due to optimization of these processes providing optimum strain hardening.

The grain size effect on crack blunting (associated with lattice dislocation emission from cracks) in nanocrystalline ceramics at elevated temperatures is theoretically speicified. The dependence of the number of dislocations emitted by a crack on grain size in nanoceramics 3C-SiC is calculated which characterizes the grain size effect on crack blunting that crucially influences ductility of this material.

A theoretical model is suggested which describes mobility of triple junctions of grain boundaries during their stress-driven migration in deformed nanocrystalline materials. Within the model, one can distinguish mobile triple junctions serving as structural elements which decrease the strength and enhance the fracture toughness of nanocrystalline ceramics.

A dislocation model is proposed which describes the strengthening effect of Y-junction nanotubes in ceramic nanocomposites. In the model, nanotubes slip along the nanotube/matrix interface through the motion of prismatic dislocation loops. When such a loop meets a Y-junction of nanotubes, it needs a critical shear stress to bypass the junction. It is shown that the critical stress increases with decreasing nanotube radius and wall thickness. Thus, the thinnest nanotubes should provide the most effective strengthening and toughening of ceramic nanocomposites with nanotubes that form Y-junctions.

Nucleation of nanograins near crack tips and its role as a special (new) toughening mechanism in deformed nanocrystalline materials are theoretically described. Within our description, stress-driven splitting and migration of grain boundaries occur near crack tips. These stress-driven processes result in nucleation of nanograins and cause a partial stress relaxation near cracks. It is shown that the nucleation of nanograins near crack tips is energetically favorable and effective in toughness enhancement in nanocrystalline ceramic alpha-Al2O3.

A new physical mechanism of plastic deformation in nanowires (either free-standing metallic nanowires or nanowire-like inclusions of the second phase in ceramic nanocomposites) is suggested and theoretically described. This mechanism represents formation of near-surface nanodisturbances – nanoscopic areas of plastic shear with tiny shear vectors – in deformed nanowires. We calculated the energy characteristics for nanodisturbance formation and compared them with those for conventional dislocation generation. It is shown that the nanodisturbance deformation mode tends to dominate in Au nanowires deformed at high stresses and zero temperature.

Two different modes of delamination in nano-alumina-titania coatings on steel substrates, which are attributed to the conventional fully-melted (FM) and the bi-modal fully-melted and partially-melted (FM-PM) coating, are discussed. Using simple theoretical models of the coating/substrate interfaces, typical for these coatings, we analyze the profits of the bi-modal FM-PM coatings over the conventional FM coatings in terms of effective specific energy of adhesion, critical strain of delamination, and critical thickness of the coating. It is shown that use of the bi-modal FM-PM coatings can lead to doubling the interface toughness and increasing the critical strain by 50% and the critical thickness by more than 130%.

Stress-induced nucleation of nanoscale grains in deformed nanocrystalline ceramics is theoretically described as a special deformation mode initiated by preceeding intergrain sliding and/or lattice slip. The nanograin nucleation occurs through splitting and migration of grain boundaries containing disclination dipoles produced by intergrain sliding and/or lattice slip.

A special mode of plastic deformation associated with athermal grain growth in nanocrystalline ceramics is theoretically described. The mode represents the stress-induced cooperative migration of grain boundaries, when the migration involves two or more neighboring boundaries. Theoretical models are suggested that describe the effects of stress-driven migration of grain boundaries on both the formation of nanoscale cracks and growth of comparatively large cracks in deformed nanocrystalline ceramics.

A theoretical model is suggested that describes the generation of deformation twins near brittle cracks of mixed I and II modes in nanocrystalline ceramics. In the framework of the model, a deformation twin nucleates through stress-driven emission of twinning dislocations from a grain boundary distant from the crack tip.

A theoretical model is suggested which describes the generation of nanoscale cracks at defect configurations formed at interfaces due to interfacial sliding in deformed nanocrystalline ceramics. A theoretical model is suggested that describes stress relaxation through local migration of interfaces in nanocrystalline ceramic, metallic and cermet coatings. It is theoretically shown that the local migration results in formation of wedge disclination quadropoles whose stress fieds compensate for, in part, mismatch stresses in nanocrystalline coatings.

A special mechanism of strain hardening in deformed nanocrystalline ceramics is suggested and theoretically described. The mechanism represents generation of disclination dipoles at interfaces (grain and interphase boundaries) due to interfacial sliding. It is shown that special strain hardening can effectively suppress plastic flow instability in nanocrystalline ceramics and thus enhance their ductility/machinability. At the same time, the disclination dipoles formed due to interfacial sliding serve as dangerous stress sources that can induce nucleation of nanocracks, decreasing ductility/machinability of nanocrystalline ceramics.

A theoretical model is suggested that describes a special microscopic mechanism for generation of lattice dislocations at amorphous intergranular boundaries in deformed nanocrystalline ceramics. In the framework of the model, a dipole of lattice dislocations is generated through a nanoscale ideal shear that occurs within an amorphous intergranular boundary and has magnitude growing continuously under the shear stress. Energy characteristics of the generation process are calculated. It is theoretically revealed that the generation process is energetically favorable and can occur in athermal way (without any energy barrier) in technologically and scientifically important nanoceramics, 3C-SiC and TiN/a-Si_3N_4, in wide ranges of their parameters. With results of the model, the dependence of the hardness on the volume fraction of the amorphous phase a-Si_3N_4 in ceramic nanocomposite TiN/a-Si_3N_4 was calculated.

An overview of experimental data and theoretical models of fracture processes in ceramic nanocomposites is presented. The key experimentally detected facts and basic theoretical representations in this area are considered. Special attention is paid to discussion of toughness enhancement mechanisms in ceramic nanocomposites.

A theoretical model is suggested that describes nucleation of cracks at grain and interphase boundaries in deformed ceramic nanocomposites with bimodal structures. In the framework of the model, cracks are generated in the stress fields of disclinations and dislocations that are formed at interfacial steps due to transfer of plastic flow across interfaces dividing adjacent crystallites of the same or different phases.

Technology Transfer

Interactions are planned with scientists from Naval Research Laboratory (Washington, DC) for transfer of data (results of theoretical models developed in the framework of the project) for their use.

Referred Journal Articles

1. I.A. Ovid'ko, N.V. Skiba, and A.K. Mukherjee, Nucleation of nanograins near cracks in nanocrystalline materials. Scripta Materialia, 62 (2010) 387-390.
2. M.Yu Gutkin, I.A. Ovid'ko, Effect of Y-tubes on strengthening of nanocomposites, Scripta Materialia, 61, N 12 (2009) 1149-1152.
3. S.V. Bobylev and I.A. Ovid'ko, Nanodisturbances in deformed nanowires, Physical Review Letters 103, N 13 (2009) 135501.
4. M.Yu Gutkin, I.A. Ovid'ko, Plastic flow in amorphous covalent solids and nanoceramics with amorphous intergranular layers, Reviews on Advanced Materials Science, 21, N 2 (2009) 139-154.
5. I.A. Ovid'ko and A.G. Sheinerman, Enhanced ductility of nanomaterials through optimization of grain boundary sliding and diffusion processes, Acta Materialia 57 (2009) 2217-2228.
6. S.V. Bobylev, A.K. Mukherjee and I.A. Ovid'ko, Emission of partial dislocations from intergranular amorphous boundaries in deformed nanocrystalline ceramics, Scripta Materialia 60, N 1 (2009) 36-39.
7. S.V. Bobylev, A.K. Mukherjee and I.A. Ovid'ko, Amorphous intergranular boundaries as toughening elements in nanocrystalline ceramics, Rev. Adv. Mater. Sci. 21, N 1 (2009) 99-105.
8. I.A. Ovid'ko and A.G. Sheinerman, Grain size effect on crack blunting in nanocrystalline materials, Scripta Materialia 60 (2009) 627-630.
9. 5. S.V. Bobylev and I.A. Ovid'ko, Mobility of triple junctions of grain boundaries during their migration in deformed nanocrystalline materials, Rev. Adv. Mater. Sci. 22 N 1/2 (2009) 39-61.
10. I.A. Ovid'ko and A.G. Sheinerman, Crack blunting through lattice dislocation slip in nanocrystalline and ultrafine-grained materials, Mater. Sci. Forum, 633-634 (2009) 55-62.
11. I.A. Ovid'ko, A.G. Sheinerman and E.C. Aifantis, Stress-driven migration of grain boundaries and fracture processes in nanocrystalline ceramics and metals, Acta Materialia 56, N 12 (2008) 2718-2727.
12. S.V. Bobylev and I.A. Ovid'ko, Nanograin nucleation initiated by intergrain sliding and/or lattice slip in nanomaterials, Appl. Phys. Lett. 92, N 8 (2008) 081914.
13. I.A. Ovid'ko and A.G. Sheinerman, Nanocrack generation at dislocation-disclination configurations in nanocrystalline metals and ceramics, Phys. Rev. B 77, N5 (2008) 054109.
14. M.Yu Gutkin, K.N. Mikaelyan and I.A. Ovid'ko, Athermal grain growth through cooperative migration of grain boundaries in deformed nanomaterials, Scripta Materialia 58, N 10 (2008) 850-853.
15. M.Yu Gutkin, I.A. Ovid'ko and N.V. Skiba, Crack-stimulated generation of deformation twins in nanocrystalline metals and ceramics, Philosophical Magazine 88,

N 8 (2008) 1137-1151.
16. I.A. Ovid'ko and A.G. Sheinerman, Special strain hardening mechanism and nanocrack generation in nanocrystalline materials, Appl. Phys. Lett. 90, N 17 (2007) 171927.
17. I.A. Ovid'ko and A.G. Sheinerman, Plastic deformation and fracture processes in metallic and ceramic nanomaterials with bimodal structures, Rev.Adv.Mater.Sci. 16, N 1/2 (2007) 1-9.
18. I.A. Ovid'ko, A.G. Sheinerman and N.V. Skiba, Stress relaxation through local migration of interfaces in nanocrystalline coatings, Rev.Adv.Mater.Sci. 16, N 1/2 (2007) 102-107.
19. M.Yu Gutkin, K.N. Mikaelyan, I.A. Ovid'ko, Enhanced interface toughness of bi-modal nano-alumina-titania coatings, Reviews on Advanced Materials Science, 26 (2010), in press.

Books and Chapters

1. Book chapter: I.A. Ovid'ko, Fracture Processes in Advanced Nanocrystalline and Nanocomposite Materials. in: "Nanoscience and Its Applications in Biomedicine", edited by Donglu Shi (Springer-Verlag and Tsinghua University Press, 2009), pp. 531-561.

2. Book chapter: I.A. Ovid'ko and A.G. Sheinerman, Fracture behavior of nanocrystalline ceramics. Chapter: in Book "Mechanical Properties of Nanocrystalline Matterials", edited by J.C.M. Li (Pan Stanford Publishing, C/o World Scientific Publishing Co., Inc., Hackensack, NJ, 2010) 33 pages, in press.

Technical Reports

None entered

Contributed Presentations

1. I.A. Ovid'ko, Plastic deformation and fracture micromechanisms in nanostructured materials (invited talk) // 1st Int. Conf. from Nanoparticles and Nanomaterials to Nanotechnologies and Nanodevices, June 16-18, 2008, Halkidiki (Greece).

2. I.A. Ovid'ko, A.G. Sheinerman. Disclination mechanism for strain hardening and nanocrack generation in nanocrystalline ceramics and metals // 11th Int. Workshop on New Approaches to High-Tech: Nano Design, Technology, Computer Simulations, September 17-21, 2007, Bayreuth (Germany).

3. S.V.Bobylev, M.Yu.Gutkin, I.A.Ovid'ko, N.V.Skiba, A.G.Sheinerman, and E.Aifantis. High-strain deformation mechanisms in nanocrystalline metals and ceramic nanocomposites. The 2nd International Symposium "Physics and Mechanics of Large Plastic Strains", June 4-9, 2007, St. Petersburg, Russia

4. M.Yu. Gutkin, I.A. Ovid'ko, N.V. Skiba. Features of twin deformation in nanocrystalline metals and ceramics // The 5th International Conference on Phase Transitions and Strength of Crystals, November 17-21, 2008, Chernogolovka (Russia).

5. M.Yu. Gutkin, I.A. Ovid'ko, N.V. Skiba. Generation of deformation twins in nanocrystalline materials near cracks. International Workshop on the Plasticity of Nanocrystalline Metals, September 28 – October 1, 2008, Lake Bostal (Germany).

Patents

None entered

Honors

None entered

Other Sponsored Work

1. Theory of Plastic Deformation and Fracture of Nanostructured Films and Coatings
   for: Russian Foundation of Basic Research (around US$ 40 K (1200 K Russian roubles))
   from: January 1, 2008 to: December 31, 2010
   The research project (with I.A. Ovid'ko being PI) is focused on a theoretical description of microdeformation and interfacial crack nucleation processes releasing residual stresses in nanostructured films and coatings.

2. Development of fundamental theory of functional properties of advanced ceramic nanocomposites
   for: Presidium of Russian Academy of Sciences (around US$ 100 K (3 M Russian roubles))
   from: January 1, 2009 to: December 31, 2011
   The research project (with I.A. Ovid'ko being PI) is focused on theoretical study of functional properties of ceramic nanocomposite materials exploited at elevated temperatures.