4th International Conference on

Condensed Matter and Materials Physics

August 16-17, 2018 | London, UK

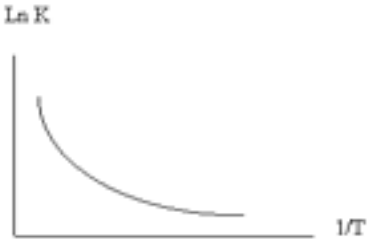
e-Posters

Anatoly V Stepanov, Res. Rev. J Mat. Sci. 2018, Volume 6
DOI: 10.4172/2321-6212-C2-018

Information entropy for transformation of molecular structure

Anatoly V Stepanov
Belorussian State University, Republic of Belarus

There are two processes for transformation of molecular structure: a high-temperature transformation (Arrhenius dependence) and molecular tunneling (low-temperature plateau). Calculation of information entropy for these processes gives us some useful information, namely probabilities of occurrence of the reactions under considerations, their efficiency and mean-square fluctuations of the distribution function parameters. Essentially, this investigation is an evolution of Perrin's radiation hypothesis proposed in 1919. Almost one century has passed…And now a fuller picture of the elementary activation act for unimolecular chemical reaction begins to emerge. Arrhenius dependence with low-temperature plateau.



Recent Publications:

1. Stepanov A.V., Stepanov M.A. (2018) Information entropy of molecular tunneling. Proceedings 2:151-162.
2. Stepanov A.V. (2015) Information entropy of activation process: Application for low-temperature fluctuations of a myoglobin molecule. International Journal of Modern Physics B 29:1550016-1-18.
3. Stepanov A.V. (2011) Modeling of metamaterials: a globular protein as a metamaterial prototype for electromagnetic-acoustic conversion at low temperatures. Proc. of SPIE 8070:807013-1-13.
4. Stepanov A.V. (2007) Activation process model: Einstein coefficients for activation barrier. Journal of Molecular Structure: THEOCHEM 805:87-90.
5. Stepanov A.V. (2002) Interaction model of thermal radiation with molecule at low temperatures: molecular tunneling. Journal of Molecular Structure: THEOCHEM 578:47-61.

Biography

Anatoly Stepanov has received his graduation of the BSU in 1976 and post-graduate studentship in the BSU 1983 - 1986.1989 up to the USSR disintegration: WATOC member; 1997 - 2000: NYAS member. Current research activity - there are a few problems in physics and chemistry that are in interest for me: an elementary activation act in solid state diffusion and chemical transformation; compensation effect in chemical kinetics; adiabatic and non-adiabatic approximation in molecules physics; dynamic properties of protein mobility; IR multi-photon absorption and photodissociation; molecular structure; molecular tunneling; prebiotic evolution; Einstein coefficients for activation barrier; low-temperature equilibrium fluctuations and functionally important motions in a globular protein; information entropy for activation process and molecular tunneling.

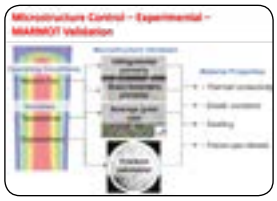
stepav@bsu.by

Jie Lian et al., Res. Rev. J Mat. Sci. 2018, Volume 6
DOI: 10.4172/2321-6212-C2-018

Advanced fuels by field assisted sintering technology: Accident tolerance and fuel performance model validation

Jie Lian, Tiankai Yao and **Bowen Gong**
Rensselaer Polytechnic Institute, USA

The advanced ceramic fuel development program is exploring revolutionary ceramic fuels with the potential of "game-changing" impact on reactor operation and response to beyond design scenario. Key properties of advanced fuels include high thermal conductivity, oxidation resistance, high temperature mechanical properties, and thus improved accident tolerance. Composite ceramic fuels possess distinct advantages to fulfill these key requirements. In addition, the US Nuclear Energy Advanced Modeling and Simulation (NEAMS) program is developing science-based next generation fuel performance modeling capability to facilitate the predictive capability of nuclear fuel performance and critical experimental data are needed to validate the multiscale multiphysics MARMOT models. In this talk, recent advancements of using field-assisted sintering technologies, specifically spark plasma sintering (SPS), in fabricating advanced fuels and engineering fuel matrix as the target systems will be reviewed. Different types of concepts are explored for the advanced fuel designs including graphene-based UO_2 composite fuels, large-grained fuel doped by oxide additive and the high uranium density fuel, and the impact on design of accident tolerant fuels were discussed. Recent progresses of using SPS in tailoring and engineering fuel matrix as the target systems for validating MARMOT physics models will also be highlighted. Particularly, monolithic oxide fuels with tailored microstructure including grain size across multiple length scales from nano-metered to micron-sizes, porosity and stoichiometry can be sintered. The impacts of tailored microstructure on thermal-mechanical properties and grain growth kinetics are discussed within the context of the MARMOT modeling.



Recent Publications:

1. Tiankai Yao et al. (2018) Radiation-induced grain subdivision and bubble formation in U3Si_2 at LWR temperature. Journal of Nuclear Materials. 498:169-175.
2. Y Miao et al. (2017) Bubble morphology in U3Si_2 implanted by high-energy Xe ions at 300°C. Journal of Nuclear Materials. 495:146-153.
3. Tiankai Yao et al. (2017) Growth and pore coarsening in dense nanocrystalline UO_{2+x} fuel pellets. Journal of American Ceramic Society. 100(6):2651-2658.
4. Yinbin Miao et al. (2017) *In situ* Synchrotron Investigation of Grain Growth Behavior of Nano-Grained UO_2. Scripta Materialia. 131:29-32.
5. Yinbin Miao et al. (2016) Correlation between crystallographic orientation and surface faceting in UO_2. Journal of Nuclear Materials. 478:176-184.

Biography

Jie Lian received his PhD degree in Nuclear Engineering & Radiological Sciences from University of Michigan in 2003 and his M.S. degree in Materials Science & Engineering from Tsinghus University at 1998 and Electrical Engineering from University of Michigan in 2001. He obtained his B.S. degree in Materials Science and Engineering from Yanshan University in China in 1995. He joined the Department of Mechanical, Aerospace & Nuclear Engineering at Rensselaer Polytechnic Institute as an Assistant Professor in 06/2008 and was promoted to Associate Professor with tenure at July 2013. He was promoted to full professor at July 2017.

lianj@rpi.edu

4th International Conference on

Condensed Matter and Materials Physics

August 16-17, 2018 | London, UK

Accepted Abstracts

Materials Physics 2018

Res. Rev. J Mat. Sci. 2018, Volume 6
DOI: 10.4172/2321-6212-C2-018

The boundary influence upon superconducting properties of high T_c superconductors

A N Lykov
P N Lebedev Physical Institute – RAS, Russia

The properties of superconducting plates with a thickness of the coherence length were investigated by numerically solving the system of one-dimensional Ginzburg-Landau-Gor'kov (GLG) equations. The new boundary condition is applied to the case of CuO_2 planes which are the main structural elements responsible for superconductivity in high T_c superconductors. Spatial dependence of the pairing potential across the thickness of the superconducting CuO_2 planes in HTSC copper oxides is found by using the GLG theory. The potential turned out to be significantly suppressed due to an effect of non-superconducting layers, which separate the CuO_2 planes. The temperature dependence of the effective energy gap was calculated in this work. The bulk interaction potential in the cuprate HTSC is estimated within the framework of BCS theory. The large value of the potential indicates the presence of a strong coupling interaction of the electrons in Cooper pairs. The effect leads to the reduction of the critical temperature of these superconductors. So that, the number of CuO_2 planes that are within a short distance of each other in unit cell should be increased for increasing T_c of the cuprate superconductors. The influence of boundary conditions in Ginzburg-Landau theory on the critical state of superconducting layered structures was studied also in the work by using new method for calculating the dependence of the critical current on the applied magnetic field. It has been shown that taking into account the influence of the boundary in the calculations leads to a better agreement with experimental data.

lykov@lebedev.ru

Res. Rev. J Mat. Sci. 2018, Volume 6
DOI: 10.4172/2321-6212-C2-018

Fluid/solid interface processes associated with emerging materials

Dimitris Drikakis and **Mike Frank**
University of Strathclyde, UK

The paper concerns processes at fluid/solid interfaces, which can lead to the design of new materials that meet specifications with regard to flow velocity, thermal conductivity and shear viscosity. In particular, the talk will focus on the effects of surface roughness on nanoflows. A fractal model is employed to model wall roughness, and molecular simulations are performed for liquid argon confined by two solid walls. It is shown that the surface roughness reduces the velocity in the proximity of the walls with the reduction being accentuated when increasing the roughness depth and wettability of the solid wall. It also makes the flow three-dimensional and anisotropic. In flows over idealized smooth surfaces, the liquid forms parallel, well-spaced layers, with a significant gap between the first layer and the solid wall. Rough walls distort the orderly distribution of fluid layers resulting in an incoherent formation of irregularly shaped fluid structures around and within the wall cavities. Furthermore, we show that while the viscosity in smooth channels remains constant across the channel width, in the presence of surface roughness it increases close to the walls. The increase of the boundary viscosity is further accentuated by an increase in the depth of surface roughness.

dimitris.drikakis@strath.ac.uk

Res. Rev. J Mat. Sci. 2018, Volume 6
DOI: 10.4172/2321-6212-C2-018

Inhibit source of 1.3 um quantum dot intermixing using STO for high laser performance

H Hashim, A Mohd and **A B Ooi**
King Abdullah University for Science and Technology, KSA

Significant behavior has been observed by studying the PL emission for post growth thermal annealing in a long wavelength QDs materials, capped with STO, highly recommended as inhibit source for intermixing, and a promising materials for highly laser performance. For intermixing studies, samples were deposited with Strontium titanium oxide (STO) 100 nm thickness using pulsed layer deposition (PLD), annealing used rapid thermal annealing (RTP) under GaAs overpressure at temperature ranging 650 to 725°C for 2 minutes were applied on it to cause thermal interdiffusion with a different rate. Samples were excited by 1064 nm laser source, and PL spectrum under 77 K were measured for all different annealing samples. Figure 1 shows a clear inhibition diffusion behavior when intermixing until 725°C annealed temperature, this gives a good reason for recommendation of this material in multiple wavelength chip, when using a mask with it, and SiO_2 as a second promote intermixing source. A strain effect clear in the deposited samples shows as a red shift in the spectra. A second observation have been seen is the merging of the two peaks, GS and first excited state, while annealing the diffusion of In in the dots cause a change in the QDs density of state, which seen as a merging in the two states, in order to estimate the critical temperature that the states have been merged, we plot the different in energy between GS, ES1 as a function of annealing temperatures- figure 2, the point where the linear line intercept with X axis represent the critical temperature. Gaussian fitting have been used to estimate the peaks wavelength for all spectrum, figure (3) shows the behaviors when annealing, for whole spectrum a decrease in FWHM has been observed while annealing until 700°C around critical temperature it started to increase (because of third peak effect), For GS behavior, it started to decrease with annealing (because of merging with ES1, above TC, it completely merge so couldn't be estimated from Gaussian fitting. For ES1: it started to increase, (cause of GS merge with it), then at TC started to decrease (because of appearance of third peak).

Hala.alhashim@kaust.edu.sa.

Res. Rev. J Mat. Sci. 2018, Volume 6
DOI: 10.4172/2321-6212-C2-018

Electrical characterization of He-ion irradiated Pd/n-SiGe Schottky diode

Mohammed Mamor[1] and **Khalid Bouziane**[2]
[1]Cadi Ayyad University, Morocco
[2]International University of Rabat, Morocco

There has been considerable interest in integrating high speed and novel devices made from $Si_{1-x}Ge_x$ materials, since the alloy is compatible with the silicon based technology. Ion implantation is now a common process in the mature semiconductor industry and is widely used during several electronic devices fabrication steps. In particular, ion implantation is used to improve the fast switches and the performance of photodiodes. Moreover, it is well known that ion implantation into semiconductor materials has a profound influence on the structural and electronics properties of their surface and subsurface region. The ion implantation induces structural and electronic changes, which governs the characteristics of metal contacts formed on the semiconductor. In this presentation, we report on the electronic properties of He-ion irradiation induced defects, as determined by deep level transient spectroscopy (DLTS). In addition, we present the results obtained on temperature-dependent of the Schottky barrier height (SBHs) fabricated on He-ion irradiated n-$Si_{0.90}Ge_{0.1}$ and the impact of this irradiation on the conduction mechanism in Pd/n-$Si_{0.90}Ge_{0.10}$ Schottky barrier diodes (SBDs). The electrical properties of He-ion irradiated Pd/n-$Si_{0.9}Ge_{0.1}$ Schottky diodes were studied in a wide temperature range (100-300 K). It was found that the current flow is controlled mainly by thermionic emission. The Schottky barrier height (Φ_{bn}) and ideality factor (n) of Pd/n-$Si_{0.9}Ge_{0.1}$ Schottky diode have been studied as a function of temperature. A decrease of Φ_{bn} and an increase of n with decreasing temperature are observed. Additionally, linear dependence between the so-called temperature factor T_0 and temperature as well the well-known linear correlation between SBHs and ideality factors, Φ_{bn} (n), are observed and explained in terms of inhomogeneities due to the presence of He-ion irradiation induced defects and traps with associated energy level localized in the gap.

mohammedmamor@yahoo.com

Res. Rev. J Mat. Sci. 2018, Volume 6
DOI: 10.4172/2321-6212-C2-018

Texture simulation of cold-rolled FCC metals by using Taylor model

Shih Chieh Hsiao
NCKU, Taiwan

The orientation of grains plays a significant role at the anisotropy of mechanical properties. In 1980s, Van Houtte proposed the revised model, as known as the relaxed constrained Taylor model, to predict the experimental rolling texture of high SFE metals. Until now, lot of researchers work on the evolution of the texture between experiment and simulation, but are not able to simulate all the specific texture simultaneously, and the intensity of them are quite different as well. Thus, in this research, we combined the full constraints and relaxed constraints Taylor models to predict the texture of severely cold-rolled copper, and compare the difference of texture between experiment and simulation quantitatively. This study consists of cold-rolling experiment and numerical simulation. In cold-rolling experiment, copper was rolled and measured by XRD and EBSD to analyze the texture and microstructure respectively. In numerical simulation, statistical 10,000 orientations were imported to the combined Taylor model to simulate the rolling texture measured by XRD. In experiment, the 95% cold-rolled copper shows high Cu (16.2%), S (34.6%) and Bs (14.4%) orientations, which are the main components of rolling texture of high-stacking-fault-energy metals. In simulation, the combined Taylor model successfully simulates high Cu (9.21%), S (23.24%) and Bs (13.81%) orientations. The results are showed as {111} pole figure in figure 1, symbol ●,▲ and ▪ stands for Cu, S and Bs respectively. The combined Taylor model is able to predict the deformed texture. Not only the preferred orientations but also the intensity are achieved.

sshawnnccatt@hotmail.com

Res. Rev. J Mat. Sci. 2018, Volume 6
DOI: 10.4172/2321-6212-C2-018

Diamond growth in air at room temperature in CVD-grown pseudo-graphite films

I M Shmytko, O V Misochko and **S K Brantov**
Institute of Solid State Physics - RAS, Russia

Attempts have been made to develop a simple and fast technique of producing diamond-like films by chemical vapor deposition (CVD) via methane pyrolysis at ~1270-1420 K using a simple reaction cell in the form of a capacitor. Under the impact of electric field ~ 10^{-2} V/μm the carbon condensed onto single crystal silicon substrates placed between the capacitor graphite plates. However, applying this technique we obtained instead of diamond-like films, pseudo-graphite films with graphitization index of ≈0.44. The films were extremely brittle, easily ground in an agate mortar into nanopowder with grain sizes of several tens of nanometers and demonstrated micro hardness comparable to that of diamond (~70-90 GPa). They also exhibited a pronounced texture in the direction of the film normal coinciding with the graphite c-axis and consisted of nanocrystallites with average size <D>≈7 nm. Moreover, the films turned out to be highly inhomogeneous with local lattice parameter variations Δc≈0.22 Å (Δc/c≈ε=3.15%). After ~ 2 years this film aged in a normal atmosphere at room temperature have undergone considerable and, in our opinion, unique variations. Researches on the film by XRD, Raman spectroscopy and SEM methods showed that for the aging their structure has changed. The main products of the interaction of the films with the atmosphere turned out to be carbide of silicon and carbon in the form of micro crystalline diamond of high perfection, see fig.1-b. The mechanism reconstruction of pseudo-graphite film into the silicon carbide and diamond is discussed.

shim@issp.ac.ru

Res. Rev. J Mat. Sci. 2018, Volume 6
DOI: 10.4172/2321-6212-C2-018

Storage capacity of clathrate hydrates for storing small molecules

Suresh Kumar, Chivukula V Sastri and **Hemant Kumar Srivastava**
Indian Institute of Technology Guwahati, India

Density functional theory (DFT) based studies are carried out to understand the structure, stability and reactivity of clathrate hydrates with or without hydrogen encapsulation. All geometries of clathrate hydrates were fully optimized using B3LYP/6-31G(d), M06-2X/6-31G(d) and B97D/6-31G(d) level of theories. The storage capability of five standard clathrate hydrates (5^{12}, $4^3 5^6 6^3$, $5^{12}6^2$, $5^{12}\ 6^4$ and $5^{12}6^8$) is systematically explored to store small molecules like Ar, CH_4, CO_2, H_2, H_2S, Kr, N_2, O_2 and Xe. The capability is depicted in the given Figure. The efficacy of trapping of small molecules inside the cages of clathrate hydrates generally depends upon the cavity sizes and shapes. The interaction energy values indicate the formation of stable gust-host system.

sureshkr@iitg.ernet.in

Res. Rev. J Mat. Sci. 2018, Volume 6
DOI: 10.4172/2321-6212-C2-018

Study of anomalous vibrational dynamics in tetrahedrite thermoelectrics by integrated computational and experimental methods

Wei Lai
Michigan State University, USA

Tetrahedrites with the general compostion of $Cu_{12-x}M_xSb_4S_{13}$ recently have emerged as promising thermoelectrics with earth-abundant and environment-friendly elements. While it has been shown that they possess favorable electronic properties and low lattice thermal conductivity (<1 W m-1 K-1 for a wide temperature range), the vibrational dynamics in this family of materials is not well-understood. In this talk, we will present some of our integrated computational and experimental efforts to study anomalous vibrational dynamics in tetrahedrites. We will first show computational results on the electron density, heat capacity, elastic moduli, and EXAFS spectra that agree with experiments. We will then focus on the role of lone-pair electrons of Sb on the vibrational dynamics, anomalous "phonon softening upon cooling", and quasi-localized vibration modes that lead to low lattice thermal conductivity.

laiwei@msu.edu

Res. Rev. J Mat. Sci. 2018, Volume 6
DOI: 10.4172/2321-6212-C2-018

Effect of process parameters on dimension of single-track ss316l deposited by direct energy deposition

Yen Ting Chen
NCKU, Taiwan

Direct Energy Deposition (DED) has been recently applied for production of complex structure and for different areas, because of its convenient feature. However, there are still lots of problems, such as how to control the process parameters to get demand cladding dimension and to improve product properties. The purpose of this research is to analyze the effect of process parameters on dimension of single-track 316L stainless steel by DED and find a prediction index of dimension control. In this study, DED experiments were carried out with powder and substrate of 316L stainless steel to investigate the influences of process parameters (Laser Power and Scan speed) on laser forming properties. Software ImageJ was used to analyze the dimensions and morphology. From our results, it was found that increase in laser power leads to increasing the cladding area, height, and width. Secondly, increase in scan speed results in the unsymmetric morphology of cladding, and in decreasing the area and height of cladding, but it doesn't have significant influence on the cladding width. Thirdly, energy index and dimension index could be used to help on controlling process parameters. When the energy index E>50, molten pool boundary expands across to the substrate and make it could be always found the re-melt zone below substrate. For dimension index DI>0.8, more powder could be deposited on the substrate (cross section area of per unit track is larger than 1.8mm2) .

qqw0x0xpp@hotmail.com