ISMANAM2007

Scientific Program
and
Book of Abstracts

14th International Symposium on Metastable and NAno-Materials

Symposium Organiser: G.A. Evangelakis

Corfu, GREECE

26th – 30

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16:50 Talk ..... DIV/O_123

A phenomenological microscopic view of chemical reactivity of nanocrystalline materials under shear

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It is well known that solid phases under far-from-equilibrium conditions display an enhanced chemical reactivity. This is the case of mechanochemical methods in which chemical potential and mechanical deformation effects are coupled. Such evidence has been widely exploited in the past to synthesize a variety of advanced and metastable materials. Despite this, a satisfactory rationalization of the above mentioned effects has not yet been attained. In this contribution we show that an accurate characterization of chemical reactivity combined with a quantitative evaluation of mechanical energy delivered to reactants under shear conditions can provide useful information on the surface activity of strained solids. This also represents a valuable tool to highlight the occurrence of mechanochemical effects. The cases of solid-solid and solid-gas reactions as well as of catalytic systems will be discussed.

17:05 Invited talk ..... DIV/IO_308

Structural aspect of the formation and properties of bulk metallic glasses

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By fitting the potential energy hypersurface derived from first-principles calculations (involving more than 500 atomic configurations), accurate embedded atom method (EAM) interactomic interactions have been obtained for multicomponent Zr-Cu-Al-Y glass formers. The as-obtained EAM interatomic potentials enable us to analyze these complex systems using computer simulation on a larger scale, both spatially and temporally. Metallic glasses were obtained by quenching the liquid at slower cooling rates using classical molecular dynamics (MD). For experimental validation, Zr-Cu based metallic glasses with different compositions and components (e.g., Zr54Cu46, Zr47Cu46Al7, Zr42Cu46Al7Y5, etc) have also been subjected to synchrotron X-ray diffraction and extended X-ray absorption fine structure (EXAFS) analysis conducted at the Advanced Photon Source. The pair correlation functions, local atomic environments, and structure factors have been found to be in agreement with that derived from MD computer simulations. The structural features of the simulated metallic glasses, in particular the size distribution of interatomic open volume (excess or free volume), have been characterized in detail. Next, a number of important physical quantities of the metallic glasses have been assessed and compared with experiments, including liquid fragility, dynamic heterogeneity, glass transition, vibrational properties, and mechanical properties (e.g., elastic constants, Poisson's ratios etc). The role of the atomic-level structure (in particular, the distribution of the loosely packed regions with larger interatomic space) in affecting the glass forming ability as well as other physical properties will be addressed.

17:25 Talk ..... DIV/O_222

Phase-field modelling of microstructural evolution in primary crystallization

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One of the main routes to obtain nanostructured materials is through the primary crystallization of glasses. In such transformations, crystallites with a different composition than the amorphous precursor grow with a diffusion-controlled regime. Particle growth is slowed and eventually halted by the impingement between the concentration gradients of surrounding particles. Primary crystallization kinetics is not well described by the KJMA equation, and this fact was generally ascribed to both the soft-impingement effect and the non-random nucleation. However, recent phase-field simulations showed that the underlying physical reason is the change in the local diffusion properties of the amorphous precursor due to the variation of the composition during the transformation [1]. The kinetics of primary crystallization is thus well described by considering a diffusion coefficient of the slowest diffusing species dependent on the local concentration [2]. The nanostructure developed in such transformations is a key point to explain the macroscopic properties of these materials. In this work the grain size distributions obtained in realistic phase-field simulations of transformations with continuous nucleation and both constant and variable diffusion coefficient are presented. The obtained distributions are analyzed and compared with theoretical distributions expected in nucleation and growth processes and the physical mechanisms responsible of their different features are recognized.

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17:40 Invited talk ..... DIV/IO_156

Rheology and ultrasonic properties of metallic glass-forming liquids: A Potential Energy Landscape approach

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In several recent studies [1-7], the flow of metallic-glass forming liquids has been modeled as configurational hopping between inherent states across energy barriers that are assumed to be on average sinusoidal. Such treatment gave rise to a functional relation between viscosity and isoconfigurational shear modulus, which led to a rheological law capable of effectively simulating the Newtonian and non-Newtonian viscosity of metallic glass-forming liquids over a broad range of fragility. In this talk, we will present rheological and high frequency ultrasonic data gathered within the supercooled liquid regions of Pt-based, Pd-based, and Zr-based glass-forming alloys. Accurate correlations between ultrasonic data and rheological data will be presented confirming the validity of the proposed treatment. Moreover, a scaling tendency between variations in shear modulus (induced either by thermal excitation or mechanical deformation) and variations in the measured stored enthalpy will be presented, verifying that the elastic softening of these materials is govern by a unique functional relation between shear modulus and configurational potential energy, a result consistent with Potential Energy Landscape theory.

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18:00 Talk ..... DIV/O_325

Vibrational properties of NiO thin film deposited on Ag(001)

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The structure and the dynamical behavior of oxide surfaces play an important role in phenomena like sintering, grain growth, oxidation, surface roughening etc [1]. NiO is a technologically interesting material for several applications: its antiferromagnetic property or its p-type semiconductivity make it candidate for applications in micro- and opto-