MM 62: Microstructure and Phase Transformations - nucleation kinetics and pressure effects

Time: Thursday 11:45–13:00 Location: IFW B

MM 62.1 Thu 11:45 IFW B

Crystallization behavior of the Al86Ni8Y6 metallic glass forming alloy upon rapid cooling — •Alexander Kuball, Moritz Stolpe, and Ralf Busch — Saarland University, Chair of Metallic Materials, Saarbrücken, Germany

In this study, the crystallization behavior of Al86Ni8Y6 upon rapid cooling from the equilibrium melt is investigated and the crystalline phases that compete with the glass formation are identified. Al86Ni8Y6 is one of the best glass formers in the ternary Al-Ni-Y system. Contrary to previous studies suggesting α-Al as the primary phase upon quenching, this study reveals that glass formation is strongly restricted by the formation of the primary precipitating ternary intermetallic compound Al23Ni6Y4. The nucleation of Al23Ni6Y4 appears to be triggered by yttrium oxide particles present in the melt acting as heterogeneous nucleation sites. Once the primary phase Al23Ni6Y4 has been formed, further crystallization of the Ni and Y depleted melt occurs as α-Al. The corresponding results are shown and discussed with respect to their effects on the glass formation.

MM 62.2 Thu 12:00 IFW B

Can homogenous nucleation be controlled in a metallic glass? — •Bin Yang[1], Yulai Gao[2], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Albert-Einstein Str. 23-24, 18051 Rostock, Germany — [2]State Key Laboratory of Advanced Special Steels, Shanghai University, 149 Yanchang Road, 200072 Shanghai, PR China

Fast scanning chip calorimetry was successfully employed to not only suppress crystallization but also bypass homogeneous nucleation of an Au-based bulk metallic glass on controlled fast quenching. A truly amorphous metallic glass without homogeneous nucleation was acquired. Following the rapid quenching, annealing at different temperatures from 0.001 s to 10000 s was realized, in which homogeneous nucleation was allowed and various local-configurations were obtained consequently. Its effect on crystallization was quantified based on the evolution of enthalpy employing Tammann's two stage nuclei development approach. Finally, a C-curve illustrating the homogeneous nucleation kinetics was obtained and added to the conventional TTT diagram, by which a truly amorphous state and the kinetics of homogeneous nucleation can be estimated. The art to control homogeneous nucleation and the science to uncover the corresponding mechanism provide new insights how to tune the micro- to nano-structure of metallic glasses, and facilitates the understanding of solidification and glass forming ability both in engineering and scientific fields.

MM 62.3 Thu 12:15 IFW B

Thin interface asymptotics in the presence of convection for diffuse interface models of solidification — •Amol Subhedar, Fathollah Varnik, and Ingo Steinbach — ICAMS, Ruhr Universität Bochum, Germany

As a major transport mechanism, convection plays a critical role in the solidification phenomena. Here, the influence of convection on diffuse interface models of solidification is investigated both analytically and via numerical simulations. It is shown that results of the diffuse interface width become independent of the auxiliary interface width, as also shown in the absence of flow (A. Karma and W. Rappel, Phys. Rev. E, 53, p. 4323 (1996)). Analytic predictions are found to be quantitatively in line with the results obtained from extensive numerical simulations for various fluid-solid coupling schemes. This underlines the generic character of the results and highlights the broad range of its applicability to various available models of solidification in the presence of flow [A. Subhedar, I. Steinbach, F. Varnik, in preparation].

MM 62.4 Thu 12:30 IFW B

High Pressure Structural Phase Transition in NdX (X=P, As, Sb): A Density Functional Theory Study — •sanjay kumar singh[1,2], rishi singh[2], and ajay mittal[3] — [1]Department of Physics, Computational Material Physics Group, Aryabhatta Group of Institutes, NH-71, Bajakhana Road, Barnala - 148101, Punjab; India — [2]Department of Physics, S. S. V. Degree College, Hapur, C. C. S. University, Meerut, India — [3]Department of Mathematics, Aryabhatta Group of Institutes, NH-71, Bajakhana Road, Barnala - 148101, Punjab; India

The structural and phase transition properties of NdX (X = P, As, Sb) under high pressure have been investigated using an ab-initio full potential linear augmented plane wave plus local orbitals approach within the framework of density functional theory as implanted in the WIEN2k package. In this approach the generalized gradient approximation is chosen for the exchange-correlation functional energy optimization for calculating the total energy. At ambient conditions NdX stabilize in NaCl (B1 phase) structure. Under compression, it undergoes first-order structural transition from Fm-3m to P4/mmm (body centre tetragonal) phase at 30.0, 24.06 and 15.1 GPa which is found to be in good agreement with the available experimental data 30.0, 24.2 and 15.0 GPa respectively. The structural properties viz., equilibrium lattice constants, bulk modulus and its pressure derivative and volume collapse are also calculated and compared with previous calculations and available experimental data.

MM 62.5 Thu 12:45 IFW B

Pressure-induced ferroelastic phase transition in SnO_2 from density functional theory — •Lei Yang, Weiliu Fan, Yanlu Li, Lei Wei, and Xian Zhao — Shandong University

We studied the high-pressure ferroelastic transition of rutile- to $CaCl_2$-type SnO_2 within density functional theory and Landau free energy theory. Softening mechanism of B_{1g} mode (order parameter Q) and the coupling mechanism between the soft B_{1g} mode and the soft transverse acoustic (TA) mode (strain ε) are clarified by calculating Landau energy map around the ground state. It is found that the Sn-O-Sn bending induced soft B_{1g} mode effectively reduces the excess energy increase caused by bond stretching, which however always leads to SnO_6 octahedral distortion. The octahedral distortion is subsequently minimized by lattice distortion strain ε, which interacts with the soft B_{1g} mode to further increase the stability of system.