MM 3: Microstructure and Phase Transformations

Time: Monday 10:15–11:45 Location: H 0106

MM 3.1 Mon 10:15 H 0106

Phase field simulations of grain boundary wetting and melting kinetics — •Venkata Sai Pavan Kumar Bhogireddy[1], Claas Hüter[1], Jörg Neugebauer[1], Oleg Shchyglo[2], Ingo Steinbach[2], and Robert Spatschek[1] — [1]Max Planck Institute for Iron Research, Düsseldorf, Germany — [2]Interdisciplinary Center for Advanced Materials Simulation, Ruhr-University Bochum, Bochum, Germany

Grain boundary premelting is known as the phenomenon that a thin melt layer can appear between two grains already below the bulk melting point, which can cause material failure. It results from a short-ranged structural interaction between the nearby solid-melt interfaces, which are induced by the overlap of the crystal structures in the sandwiched melt. The classical prediction for the transition between wetting and non-wetting states at the melting point is $2\sigma_{sl} = \sigma_{gb}$, where σ_{sl} is the solid-melt interface energy and σ_{gb} the dry grain boundary energy. Here we report on theoretical and numerical investigations of this phenomenon using a multi-order parameter phase field model based on obstacle potentials. We find that the premelting transition is in agreement with the classical expectation, and the short-ranged interactions are predicted.

Beyond this static perspective we report on the kinetics of grain boundary melting along dry and overheated low angle grain boundaries. A steady state regime for the diffusion limited growth is found in the phase field simulations, and the melting velocity depends on the aforementioned short-ranged structural interactions. The velocities are qualitatively in agreement with a sharp interface theory.

MM 3.2 Mon 10:30 H 0106

Influence of short-range forces on melting along grain boundaries — •Claas Hüter[1], Fabian Twiste[1], Efim A. Brener[2], Jörg Neugebauer[1], and Robert Spatschek[1] — [1]Computational Materials Design Department, Max-Planck Institut für Eisenforschung, Düsseldorf, Germany — [2]Peter-Grünberg-Institut 2, Forschungszentrum Jülich, Jülich, Germany

In metallurgical processing, elevated temperatures and reduced local transition temperatures can lead to phenomena of grain boundary induced failure, as e.g. hot cracking. We introduce a model which couples diffusional melting and nanoscale structural forces in a combined nano-mesoscale sharp-interface description. We obtain analytic and numerical solutions for melting processes at grain boundaries influenced by structural disjoining forces, focusing on the experimentally relevant regime of small deviations from the melting temperature. Though spatially limited to the close vicinity of the tip of the propagating melt finger, the influence of the disjoining forces yields a strong modification of the penetration velocity. Close to equilibrium the atomistic effects near the triple junctions can be expressed through a contact angle renormalization in a mesoscale formulation. For higher driving forces, significantly higher melting velocity than predicted from a purely mesoscopic description are found.

MM 3.3 Mon 10:45 H 0106

Ab initio interpretation of the abnormal carbon redistribution during martensitic transformation in Fe-C alloys — •Xie Zhang[1,2], Tilmann Hickel[1], Jutta Rogal[2], Ralf Drautz[2], and Joerg Neugebauer[1] — [1]Max-Planck-Insitut für Eisenforschung GmbH, Düesseldorf, Germany — [2]ICAMS, Ruhr-Universität Bochum, Bochum, Germany

As a key feature of the martensitic transformation in Fe-C alloys, the abnormally low tetragonality resulting from the C redistribution is a historically pending problem. To address this issue, we developed an atomistic model for the martensitic transformation in Fe-C alloys and calculated the corresponding minimum energy paths with ab initio nudged elastic band simulations. Our insights provide a theoretical evidence for the C redistribution into different octahedral sublattices in martensite, and thus nicely explain the occurrence of the abnormally low tetragonality. It also allows us to interpret the mechanism for the martensitic transition as a combination of a tetragonal cell deformation and atomic shuffling and thus our understanding of the microstructure evolution in steels.

MM 3.4 Mon 11:00 H 0106

Atomistic simulation of the martensitic phase transition in the iron-nickel system — •Emilia Sak-Saracino and Herbert M. Urbassek — Physics Department and Research Center OPTIMAS,Erwin-Schrödinger-Straße, 67663 Kaiserslautern, Germany

Nickel is one of the most important alloying elements in steel manufacture because of its slow rate of oxidation at room temperature and also as a material for ultra-high-strength steels where the strength does not originate from carbon interstitials, but from inter-metallic compounds. By using molecular dynamics simulation, we investigate the behavior of the martensitic phase transition in the iron-nickel system. We observe this transition by imposing a heating/cooling cycle on the system and monitoring the hysteresis of the system volume with temperature. In addition we report the change of the lattice constant and of the average cohesive energy as a function of nickel content.

MM 3.5 Mon 11:15 H 0106

Localizing sources of acoustic emission during the martensitic transformation — •Robert Niemann[1,2], Jaromír Kopeček[3], Oleg Heczko[3], Jan Romberg[1], Ludwig Schultz[1,2], Sebastian Fähler[1,2], Eduard Vives[4], Lluís Mañosa[4], and Antoni Planes[4] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Technische Universität Dresden, Department of Physics, Institute for Solid State Physics, 01062 Dresden, Germany — [3]Institute of Physics, Academy of Science of the Czech Republic, Na Slovance 2, 182 02 Prague, Czech Republic — [4]Departament d'Estructura i Constituents de la Matèria, Facultat de Física, Universitat de Barcelona. Diagonal 647, 08028 Barcelona, Catalonia, Spain

Acoustic avalanches are a feature of solids under stress e.g arising from martensitic phase transitions. Local sources of acoustic emission are studied in order to enlight the microscopic mechanisms. From two-dimensionally resolved acoustic emission measurement and simultaneous optical observation of the surface we identify microstructural events at the phase boundary that lead to acoustic emission [1]. A resolution in the 0.1 mm-range was reached for the location of acoustic emission sources on a Ni-Mn-Ga polycrystal. The acoustic activity and the size distribution of the microstructural transformation events exhibit power-law behavior. The origin of the acoustic emission are elastically incompatible areas, such as differently oriented martensitic plates and grain boundaries in proximity to transforming grains. We propose a model to explain the decrease of the critical exponent in mechanical or magnetic fields. [1] Phys. Rev. B. 89, 214118 (2014)

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