MM 2: Topical Session Interface-Dominated Phemomena - Moving Interfaces / Functional Properties

Time: Monday 11:15–12:45 Location: H8

MM 2.1 Mon 11:15 H8

Theory and modeling of the austenite-martensite interface structure and glissile transformation in steels — •Francesco Maresca[1] and William Curtin[2] — [1]University of Groningen, Groningen, Netherlands — [2]EPFL, Lausanne, Switzerland

The austenite-martensite (fcc-bcc) transformation controls the formation of microstructures in a wide range of high strength steels. Recent progress in the physical metallurgy of steels has shown that nanolaminate austenite/martensite microstructures contribute to high material toughness and resistance to hydrogen-embrittlement. Despite its relevance for applications, there is no established theory for the transformation capable to predict the contribution of the austenite-martensite phase transformation to ductility. To clarify the mechanism of transformation, we have performed atomistic simulations of the interface reproducing the major experimental TEM and HRTEM observations in Fe alloys. The atomistic model reveals for the first time the structure and motion of the athermal and glissile fcc austenite/bcc martensite interface in steels. The interface structure consists of [-101](111)fcc screws, as envisioned by previous theories, and [1-11](-101)bcc screws with kinks, which was not envisioned before. The atomistic findings have guided the formulation of a new, parameter-free double-shear predictive theory of martensite crystallography. Theory predictions show that the fcc/bcc lattice parameter ratio is the key factor controlling the shape deformation (i.e. the in-situ transformation strain), which can achieve more than 90%, namely three times the existing experimental estimates. The theory can be used to guide design of tougher AHSS.

MM 2.2 Mon 11:30 H8

Atomistic simulation of grain boundary phases and transitions in fcc metals — •Tobias Brink and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Grain boundaries (GBs) can be treated as interface phases (also called "complexions") with different thermodynamic excess properties. Congruent phase transitions in pure metals—where the macroscopic GB parameters remain constant—are hard to observe experimentally, but GB phases with distinct atomic structures could recently be identified in a copper tilt GB (Meiners et al., Nature 579, 2020). It remains an open question if such phases are specific to this copper GB or a more general feature of fcc metals. Using molecular dynamics computer simulations, we investigated both Cu and Al ⟨111⟩ tilt GBs with different misorientations to verify if the copper GB phases can indeed be generalized. We furthermore used simulations with Lennard-Jones pair potentials to determine how much materials physics needs to be included in the model to recover the phases of the more realistic potentials. Recurring structural motifs appeared in all of these systems, but we found that the actual material strongly influences which phases occur and their stability. This probably excludes the possibility of deriving simple rules for the atomic structure of GB phases.

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MM 2.3 Mon 11:45 H8

Simulations of a fs laser induced A7 to sc transition in antimony — •Bernd Bauerhenne[1,2], Felipe Valencia[3], and Martin E. Garcia[1,2] — [1]Theoretische Physik - Universität Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany — [2]Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), Heinrich-Plett-Strasse 40, D-34132 Kassel, Germany — [3]Physics Department, Universidad Nacional de Colombia, Edificio 404, Ciudad Universitaria, Bogota, Colombia

We simulated the fs laser excitation of a 50 nm thick free standing antimony film using more than 4 million atoms. In our simulations, we condidered the laser-induced changes of the potential energy surface and the effects of the incoherent electron-phonon collisions - the electron-phonon coupling - into account. To do so, we derived an electronic temperature (Te) dependent interatomic potential for antimony. For this, we fitted forces and energies obtained from ab-initio MD simulations of a thin antimony film at increased Te. Furthermore, we calculated the Te-depend electron-phonon coupling constant for antimony ab-initio. In our large-scale MD simulations, we observed a laser induced A7 to sc like transition at moderate intensities. If the excitation intensity is further reduced, the transition starts at the surface and moves to the center of the film. In addtion, we analyzed the influeces of the laser-induced changes of the potential energy surface and of the electron-phonon coupling on the transition.

MM 2.4 Mon 12:00 H8

Nanoscale Friction Under Active Control in Systems With Tailored Degrees of Freedom — •Niklas A. Weber[1], Miru Lee[2], Richard L.C. Vink[1], Matthias Krüger[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

In this project, we use lateral force microscopy to investigate how friction of manganite films can be controlled by the properties of the surrounding materials. Specifically, we use phase transformations [1,2] and superlattice thin film samples [3] to actively control the film properties while keeping the surfaces unchanged.

We observed an increase in friction during resistive switching of a $La_{0.55}Ca_{0.45}MnO_3$ film [1] and during heating of a $La_xSr_{1-x}MnO_3$ thin film through the metal-insulator phase transformation [2]. Careful consideration of the different contributions and comparison with literature lead to the conclusion that the electronic contributions are not sufficient to account for our observations and make phononic contributions a promising candidate.

To test our hypothesis, we have started to perform measurements on $LaMnO_3/SrMnO_3$ superlattice systems in which the propagation of phonons can be actively manipulated by the layer spacing [3], while the morphology of the surface layer remains unchanged.

[1] H. Schmidt et.al., Phys. Rev. Mater. 2020, 4, 113610.
[2] N. A. Weber et.al., Adv. Sci. 2021, 2003524.
[3] D. Meyer et al., arXiv:2009.14532v3.

MM 2.5 Mon 12:15 H8

Interplay of domain structure and phase transitions in ferroelectric $BaTiO_3$ — Madhura Marathe, Ruben Khachaturyan, Yijing Yang, and •Anna Grünebohm — ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

Domain walls and phase boundaries are fundamental ingredients of ferroelectrics and strongly influence their functional properties. Although both interfaces have been studied for decades, often only a phenomenological macroscopic understanding has been established and it is now timely to revisit nucleation and the coupling of domains and phase transitions on an atomistic level [1]. We study domain walls in $BaTiO_3$ by means of molecular dynamics simulations based on the effective Hamiltonian approach [2]. We show that domain walls may promote the tetragonal to orthorhombic phase transition [3] and can act as nucleation centers.

[1] A. Grünebohm et al., Interplay of domain structure and phase transitions: theory, experiments and functionality, (2021).
[2] Nishimatsu et al., Phys. Rev. B 78, 104104 (2008).
[3] A. Grünebohm and M. Marathe, Phys. Rev. Mater. 4, 114417 (2020).

MM 2.6 Mon 12:30 H8

Optical properties of 3D nanosponge models created by phase-field simulations — •Malte Grunert[1], Sebastian Bohm[1], Hauke Lars Honig[1], Dong Wang[1], Jinhui Zhong[2], Peter Schaaf[1], Christoph Lienau[2], and Erich Runge[1] — [1]Technische Universität Ilmenau, Germany — [2]University of Oldenburg, Germany

We present an efficient method for the numerical creation of three-dimensional nanoporous sponge models with specified geometric properties. Such nanoporous structures can be manufactured with different geometric properties and exhibit fascinating optical properties [1,2]. We show how phase-field simulations can be used to obtain nanoporous structures with predefined optical and structural characteristics. The sponge geometries generated in this way show excellent similarity to experimentally produced sponges and the averaged geometric properties are comparable. In addition, the optical properties such as the absorption and scattering cross sections are similar. The computer-generated

sponges also exhibit experimentally confirmed optical properties such as strong spatial localization of fields and the associated strong local field enhancement.

[1] G. Hergert, J. Vogelsang, F. Schwarz, D.Wang, H. Kollmann, P. Groß, C. Lienau, E. Runge and P. Schaaf, *Long-lived electron emission reveals localized plasmon modes in disordered nanosponge antennas*, Light: Science & Applications **6**, e17075 (2017).

[2] J. Zhong et al., *Nonlinear plasmon-exciton coupling enhances sum-frequency generation from a hybrid metal/semiconductor nanostructure*, Nature Communications **11**, 1464 (2020)