MM 60: Microstructure and Phase Transformations III

Time: Thursday 15:45–17:00 Location: H39

MM 60.1 Thu 15:45 H39

Mechanically driven BCC to BCT phase transformation during wire drawing conditions of pearlitic steel: An ab initio guided model — •Gh. A. Nematollahi[1], S. Djaziri[1], Y. Li[1], C. Kirchlechner[1], B. Grabowski[1], S. Goto[1,2], D. Raabe[1], G. Dehm[1], and J. Neugebauer[1] — [1]Max-Planck Institut für Eisenforschung, D-40237 Düsseldorf, Germany — [2]Department of Materials Science and Engineering, Faculty of Engineering and Resource Science, Akita University, Tegata Gakuencho, Akita 010-8502, Japan

Cold-drawn pearlitic steel wires revealing ultra-high tensile strengths of up to 7 GPa are the world*s strongest bulk materials. Experimental observations reveal that cementite gradually decomposes during wire drawing. The C atoms resulting from the cementite decomposition are mechanically alloyed into the ferrite phase and accommodated in trapping sites around defects, such as dislocations. Surprisingly, there is also a high oversaturation of the bulk ferrite phase and experiments indicate a transformation to a tetragonally distorted system.In this work, a new ab initio informed model has been developed to take into account the strain-induced interaction of C with the host matrix as characteristic for wire drawing conditions. Our model captures the effect of the applied strain * exerted by the wire drawing process * within a renormalized C formation energy obtained by density functional theory calculations. Applying the model we demonstrate that the experimentally observed tetragonal distortion is due to a mechanically driven phase transformation from the body-centered-cubic (bcc) to the body-centered tetragonal (bct).

MM 60.2 Thu 16:00 H39

First-principle study of phase transformations in Ni_2MnGa alloy — •Martin Zeleny[1,2], Alexei Sozinov[3], Ladislav Straka[4], and Oleg Heczko[5] — [1]Institute of Materials Science and Engineering, NETME Centre, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [2]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [3]Material Physics Laboratory, Lappeenranta University of Technology, Savonlinna, Finland — [4]Aalto University School of Engineering, Laboratory of Engineering Materials, Aalto, Finland — [5]Institute of Physics of Academy of Sciences of the Czech Republic, Prague, Czech Republic

Transformation path between different phases of Ni_2MnGa alloy has been investigated using first-principle electronic structure calculations. We used the projector-augmented wave method for the calculations of total energies and stresses along the transformation paths. These include transformation from austenite (A) to nonmodulated tetragonal martensite (NM), transformation from modulated martensites (10 M and 14 M) to NM martensite, as well as transformation between adjacent twin variants of NM phase. All transformations are induced by applying external shear strain. The results show the same barrier equal to 0.4 mRy/atom for A→NM transformation, 10M→NM transformation and NM twin reorientation whereas 14M→NM transformation exhibits smaller barrier equal to 0.25 mRy/atom. Calculated lower barrier well corresponds to experimental finding that the transformation from 10M to NM always proceeds via intermediate 14M phase.

MM 60.3 Thu 16:15 H39

Martensitic phase transformation of $Fe_{70}Pd_{30}$ ferromagnetic shape memory alloy thin films due to laser shock peening — •Alina J. Bischoff[1], Ariyan Arabi-Hashemi[1], Martin Ehrhardt[1], Pierre Lorenz[1], Klaus Zimmer[1], and Stefan G. Mayr[1,2] — [1]Leibniz-Institut für Oberflächenmodifizierung, Leipzig — [2]Fakultät für Physik und Geowissenschaften, Universität Leipzig

The fcc-fct martensitic phase transformation induced by laser shock peening is analyzed in $Fe_{70}Pd_{30}$ ferromagnetic shape memory alloy thin films. At shockwave pressures of up to 2.5 GPa, X-ray diffraction and scanning electron microscopy measurements reveal formation of martensitic variants with preferred orientation of the shorter c-axis perpendicular to the surface plane. Consequential merging of growth islands on the film surface is observed. For a better understanding of the atomistics of these findings, twin boundary formation, which is characteristic of martensitic transition, as well as material shape change are further explored by classical molecular dynamics simulations.

MM 60.4 Thu 16:30 H39

Density functional theory investigation of elastic properties and martensitic transformation of Ti-Ta alloys — •Tanmoy Chakraborty, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr- Universität Bochum, 44780 Bochum, Germany

Ti-Ta alloys are considered as promising materials for high temperature shape memory alloys as well as biomedical applications. The properties of these alloys have been shown to be strongly composition dependent. The temperature for the martensitic transformation between the high temperautre cubic austenite and the low temperature orthorhombic martensite decreases linearly with increasing Ta content. Likewise, the elastic properties show clear trends with changing composition. We use density functional theory to investigate the involved phases in Ti-Ta where the disordered phases are treated by special quasi-random structures. To compare the stability of the involved phases as a function of temperature we calculate free energies using the quasi-harmonic Debye model. The obtained trends in the stability are consistent with experimentally measured transformation temperatures. Furthermore, we determine elastic properties which are in good agreement with experimentally observed trends.

MM 60.5 Thu 16:45 H39

Formation of interface layers in dissimilar Al-Cu FSW-Joints — •Roland Marstatt[1], Markus Krutzlinger[2], Johannes Luderschmid[1], Ferdinand Haider[1], and Michael F. Zaeh[2] — [1]Lehrstuhl fuer Experimentalphysik I, Universitaet Augsburg, Germany — [2]Institut fuer Werkzeugmaschinen und Betriebswissenschaften, Technical University of Munich, Garching, Germany

Friction Stir Welding (FSW) is a suitable technology to join dissimilar materials, in contrast to fusion welding processes without exceeding the solidus temperature. As a consequence, high quality joints can be produced with a minimum of deleterious intermetallic phases. Due to the process conditions, FSW seems to be a good choice to form dissimilar joints as e.g. between aluminium and copper. Process optimization aims on high quality dissimilar joints with a minimum of deleterious intermetallic phases. But still an intermetallic layer at the bonding interface is detected. However, a comprehensive description of the effective joining mechanisms is still a subject of ongoing research.

In this study the analysis of the formation of nano-scaled intermetallic layers at the bonding interface is presented. These layers play a key role for the joining mechanism and influence mechanical properties and conductivity. Therefore, dissimilar lap joints of aluminium and copper with the pin stirring in aluminium only have been investigated. The thickness of the intermetallic layer highly depends on the process temperature which varies with different process parameters. Understanding the relevant process parameters for the formation of the interlayer allows to control the joint quality. *Supported by the DFG (SPP1640).*