MM 39: Structural Materials (Steels, light-weight materials, high-temperature materials)

Sessions: Advanced steels; High temperature compounds

Time: Thursday 15:00–17:45 Location: H45

MM 39.1 Thu 15:00 H45

Impact of Ferritic, Pearlite and Martensitic Micro-structured Steels and Geometric Length Scales on Micro Tensile Testing — •Jonas Kutschmann[1,2], Thomas Pretorius[2], Andreas Offergeld[2], Andreas Kern[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, Westfälischen Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster — [2]thyssenkrupp Steel Europe AG, Kaiser-Wilhelm-Straße 100, D-47166 Duisburg

Mechanical properties of different microstructures of steels are characterized by micro tensile tests and compared to other mechanical testing methods. Out of the heavy plates, provided by thyssenkrupp, miniaturized specimens with a dog-bone shape contour were cut. The specimen dimensions are of constant gauge length of 4 mm, with a gauge width between 0.3 mm and 0.5 mm and a gauge thicknesses between 1.5 mm and 0.05 mm. The depth profile of the heavy plates are correlated to mechanical properties. The thickness of the specimens has been varied over a considerable range to verify an occurring specimen size effect.

The tensile test results are correlated to Vickers hardness measurements, average grain sizes by EBSD and macro tensile tests for the ultimate tensile strength. All steels show a linear correlation between Vickers hardness and tensile strength. Micro testing of the steels reproduce the macro-scale results well. The tensile strength is almost unaffected by down-scaling of the thickness for small grain sizes. In contrast, the fracture strain decreases together with decreasing dimension.

MM 39.2 Thu 15:15 H45

High Temperature Chlorine Corrosion - Influence of additives on alkali-capture and the effect on corrosion in waste to energy plants — •Sebastian Pentz[1], Daniel Ott[1], Ferdinand Haider[1], and Ragnar Warnecke[2] — [1]Universität Augsburg, Institut für Physik, 86159 Augsburg — [2]Gemeinschaftskraftwerk Schweinfurt GmbH, 97424 Schweinfurt

High temperature corrosion especially in waste-to-energy-plants leads to massive problems. At prevalent temperatures around 400°C-600°C corrosion is mainly chlorine induced. Responsible for the supply of chlorine at heat exchangers like superheaters or boiler walls is in majority a local release of chlorine through sulfation of solid alkali chlorides out of deposits on the steel parts. This reaction requires an atmosphere containing SO_2, H_2O, O_2 and releases HCl/Cl_2.Due to additive addition in the incinerator one tries to minimize this deposit built up. While encapturing alkalies by additives the formation of alkali chlorides is reduced which leads to less condensation of gaseous alkali chlorides on colder steel parts and therefore a reduction of chlorine enriched deposits. One possible material class for alkali-capture seem to be aluminum silicates. The interstratification of alkalies out of alkali chlorides into aluminium silicates leads to a release of chlorine. The corrosive attack of the steel through chlorine strongly depends on the released chlorine species. HCl is much less critical than Cl_2. Principles of the reaction conditions in waste-to-energy-plants are shown and laboratory experiments regarding the additive influence on kinetics of sulfation reactions and the corresponding chlorine attack are presented.

MM 39.3 Thu 15:30 H45

Theoretical modeling of interstitial carbon impurities in Fe-Mn paramagnetic alloys — Alena Ponomareva[1], Bobur Mukhamedov[1], and •Igor Abrikosov[1,2] — [1]Materials Modeling and Development Laboratory, National University of Science and Technology "MISIS", 119049 Moscow, Russia — [2]Department of Physics, Chemistry, and Biology (IFM), Linköpings University, SE-58183 Linköping, Sweden,

We present a generalization of a model that takes into account the magnetic disorder of paramagnetic host with interstitial point defects [1] towards the case of the alloys. In the framework of disordered local moment picture combined with magnetic sampling method, we calculate a solution enthalpy of carbon impurity in the paramagnetic fcc Fe-Mn steels. First, we use the magnetic special quasirandom structure (M-SQS) method for simulation of the paramagnetic state in Fe-Mn alloys without impurity. Here, Fe and Mn atoms are randomly distributed at the sites of a supercell. Next, to calculate the energies for various magnetic realizations around the interstitial carbon impurity, we move the position of the impurity within the SQS. Our calculations show that in alloys containing about 20 at. % Mn, the solution enthalpy of carbon reduces compared to the pure fcc-Fe. By analyzing the local and global effects of impurity on the properties of the matrix, we discuss various factors that could increase the carbon solubility in high-manganese austenitic steels.

[1] A. V. Ponomareva, Yu. N. Gornostyrev, and I. A. Abrikosov, Phys. Rev. B 90, 014439 (2014).

MM 39.4 Thu 15:45 H45

Quantum-mechanical study of thermodynamic and magnetic properties of disordered Fe-Al phases with vacancies — •Ivana Miháliková[1,2], Martin Friák[1,2], David Holec[3], Nikola Koutná[1,2,4], and Mojmír Šob[5,1,6] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic — [3]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, Austria — [4]Institute of Materials Science and Technology, TU Wien, Vienna, Austria — [5]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [6]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Iron aluminides have a great potential to substitute stainless steels in high temperature applications because of excellent chemical resistance to corrosion, reasonable strength and low material cost. We perform quantum-mechanical calculations to examine the thermodynamic and magnetic properties of disordered α-phase Fe-18.75 at.%Al with vacancies, using density functional (DFT). In order to reveal the relations between magnetic and structural properties of the α-phase on one hand and the distribution of atoms on the other, three different models of special quasi-random structure (SQS) were used. The properties of phases and, in particular, local magnetic moments of the Fe atoms are found to sensitively depend on the number of Al atoms in the 1st and 2nd nearest neighbor shell of Fe atoms.

45 min. break

MM 39.5 Thu 16:45 H45

Atomic force microscopy based electrical characterization of multiphase intermetallic TiAl alloys — •Markus Kratzer[1], Michael Huszar[1], Lisa Tengg[2], Helmut Clemens[2], Svea Mayer[2] und Christian Teichert[1] — [1]Institute of Physics, Montanuniversitaet Leoben, 8700 Leoben, Austria — [2]Department of Physical Metallurgy and Materials Testing, Montanuniversitaet Leoben, 8700 Leoben, Austria

Atomic force microscopy - a powerful tool for the characterization of surface morphologies on the meso- and nanoscale - is also applicable for the investigation of local microscale electrical properties. This is demonstrated for an intermetallic TiAl alloy. Due to their high creep resistance, low density, and high specific strength TiAl alloys are promising materials for high-temperature structural parts in advanced propulsion systems. However, besides the mechanical parameters also the electrical behaviour of the alloys and its constituting phases are of importance. For example, the electrical homogeneity of the material is of interest for the proper interpretation of the results form electrical test procedures like, e.g., eddy current testing. TiAl samples comprising three different crystallographic phases were investigated utilizing Conductive Atomic Force Microscopy (C-AFM) to reveal local conductivity variations on the surface. Complementary, local differences in the work function were mapped using Kelvin Probe Force Microscopy (KPFM). Local current-to-voltage characteristics of the existing micrometer sized phases, recorded by C-AFM, indicated significant differences in the electrical conductivity between the individual phases.

MM 39.6 Thu 17:00 H45

Magneto-crystalline anisotropy and magnetostriction of

Fe_2Ti — •Agnieszka L. Kozub[1,2], Alexander B. Shick[2], and Dominik Legut[3] — [1]Universität Paderborn, Paderborn, Germany — [2]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [3]IT4Innovations National Supercomputing Center VSB - Technical University Ostrava, Ostrava, Czech Republic

In comparison to the classical ferromagnets, the studies of magnetostriction of antiferromagnets are limited and gained recent attention. In this work we present a theoretical study of magnetic properties of Fe_2Ti, an antiferromagnet which crystallize in hexagonal C14 Laves phase. Calculations were performed in the framework of the density functional theory using generalized gradient approximation. We focus on magnetic properties of the compound, i.e. to determine its magnetic structure, and to compute magneto-crystalline anisotropy. From the magnetic anisotropy dependence of the lattice strain we estimate magnetostrictive coefficients. Finally, we investigate the effect of under- and over- stoichiometric composition of $Fe_{100-x}Ti_x$ on the magnetostriction.

MM 39.7 Thu 17:15 H45

A quantum-mechanical study of thermodynamic and mechanical stability of Heusler-based Fe_2AlCo polymorphs — •Martin Friák[1], Sabina Oweisová[1,2], Jana Pavlů[3,2,1], David Holec[4], and Mojmír Šob[2,1,3] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — [3]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [4]Department of Materials Science, Montanuniversität Leoben, Leoben, Austria

We use quantum-mechanical calculations to test a hypothesis of Grover *et al.* (J. Mag. Mag. Mater. 15 (1980) 699) that Co atoms in the Fe_2AlCo compound have on average 3 Fe and 3 Co atoms in their second nearest neighbor shell. We have simulated four structural configurations of Fe_2AlCo including the full Heusler structure, inverse Heusler polymorph and two phases matching this idea. The highest thermodynamic stability at T = 0 K is indeed predicted for one of the phases with the distribution of atoms according to Grover and coworkers. However, small energy differences among three of the studied polymorphs lead to a disordered B2-like phase at elevated temperatures. The fourth variant, the full Heusler phase, is predicted to be mechanically unstable. All studied variants are predicted to be ferromagnetic but local magnetic moments of Fe and Co atoms sensitively depend on the composition of the first and second coordination shells. For details see Materials 11 (2018) 1543, doi: 10.3390/ma11091543.

MM 39.8 Thu 17:30 H45

The surface and interface structures in nanofiber-reinforced ceramic matrix composites — •Yanhui Zhang and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, Dublin, Ireland

Surfaces and interfaces are active sites for chemical reactions, stress/strain concentration and defect accumulation. Efficiently engineering them is critical for the R&D of novel composites in the industry sectors of aerospace, automotive and energy & power. Interfacial parameters are often inaccessible by experimental measurements due to the nano-scale of interface regions. Given the importance of surface morphology on the interface adhesion and mechanical responses, we firstly examine by first-principles thermodynamics the stable surfaces of the promising ceramic matrix materials TiB2, ZrB2 and HfB2. Thereafter, we took at one specific ceramic matrix composite, namely graphene-reinforced ZrB2, to systematically explore the structural, energetic and mechanical characters of heterophase interfaces. We demonstrate that the surface chemistry of the ZrB2 matrix material largely shapes the interface structures (Zr-C-Zr or B-C-B) and the nature of the interfacial interactions. Interestingly, the mechanical responses of strong Zr-C-Zr interfaces are significantly influenced by the corrugation of graphene; while the B-C-B interfaces with relatively weak pi-pi stacking show similar attributes as the 2D materials during interfacial cleavage and slip. Those results provide insights into the interface bonding mechanisms in graphene/ceramic composites, and emphasize the prospect of interface engineering via surface chemistry.