

MM 49: Structural Materials (Steels, light-weight materials, high-temperature materials) - I

Time: Thursday 10:15–11:30

Location: BAR 205

MM 49.1 Thu 10:15 BAR 205

First principles study on hydrogen behaviour in Cr and Mn containing carbides of high Mn steels — ●LEKSHMI SREEKALA, TILMANN HICKEL, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237, Düsseldorf

Understanding hydrogen-assisted embrittlement of advanced high-strength steels is decisive for their application in automotive industry. Since the addition of Cr to the composition of high-Mn steels improves their corrosion resistance and simultaneously changes the microstructure, the influence of Cr and Mn on hydrogen solubility in the context of carbide formation is scientifically challenging. Density functional theory based calculations have been employed to determine the thermodynamic driving force for the formation of carbides as a function of the chemical composition of the alloy and also to study hydrogen interaction of carbides and interfaces containing Cr and Mn. Our results show that Cr has an indirect impact on hydrogen, since it strongly influences the thermal stability of the carbides like cementite and $Fe_{23}C_6$. However, the individual Cr atom interacts only weakly with H. On the other hand, Mn has a weaker impact on carbide formation. However, its incorporation into the carbides yields a remarkably strong non-linear interaction with hydrogen, qualitatively different from the known H-Mn interaction in the austenitic steel matrix.

MM 49.2 Thu 10:30 BAR 205

Interaction of helium, self-interstitial atoms and vacancies with YTiO clusters in bcc Fe — ●MUTHU VALLINAYAGAM^{1,2}, MATTHIAS POSSELT¹, and JÜRGEN FASSBENDER^{1,2} — ¹Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden, Germany — ²Technische Universität Dresden, 01062 Dresden, Germany

In nanostructured ferritic/martensitic Fe-Cr alloys YTiO clusters act as sinks for the irradiation-induced defects He, self-interstitial atoms (SIA), and vacancies (v). In this manner, irradiation swelling can be retarded significantly. In this ab-initio simulation work, interactions of He and other defects with YTiO cluster in bcc Fe are investigated considering cluster structures studied in a previous work[1]. It is found that the most stable position of He is in the center of the cluster, then interfacial vacant sites and other interstitial positions between metal or oxygen atoms, and sites away from the cluster[2]. Calculations on the addition of two and three He atoms to the cluster show that the total binding energy is equal to the sum of binding energies of individual He atoms. Therefore, He trapping depends mainly on the availability of regions with low electron density. A significant attraction between cluster and SIA is observed. This results in annihilation of SIA due to the existence of interfacial vacant sites. Vacancies are also trapped by YTiO clusters and their binding energy increases if the vacancy approaches O terminated sites. [1]Vallinayagam et al 2019 J. Phys.: Condens. Matter 31 095701 [2]Vallinayagam et al 2019 J. Phys.: Condens. Matter 31 485702

MM 49.3 Thu 10:45 BAR 205

Effect of Re and Os on the $1/2 < 111 >$ dislocations in W — ●APARNA P. A. SUBRAMANYAM, THOMAS HAMMERSCHMIDT, and RALF DRAUTZ — ICAMS, Ruhr Universität-Bochum, Bochum, Germany

W is the prime candidate for plasma facing first wall material in fusion reactors. The neutron bombardment causes nuclear transmutation of W atoms to Re and Os atoms which affect the mechanical properties of the material. In order to understand these effects, we perform large-scale atomistic simulations with a recently developed analytic bond-order potential (BOP) for the ternary W-Re-Os system. This

tight-binding based BOP provides a robust description of the underlying electronic structure and is validated against available experimental and ab-initio data. Here, we discuss the effects of Re and Os on the energetics and local atomic structure of the $1/2 < 111 >$ edge and screw dislocations in W. We also analyze the motion of these dislocations in pure W as well as in W-Re and W-Os alloys in terms of Peierls stresses and discuss the influence of these elements on the kink pair formation energy in W.

MM 49.4 Thu 11:00 BAR 205

Effect of additive materials on chlorine induced high temperature corrosion in waste-to-energy plants — ●SEBASTIAN PENTZ¹, FERDINAND HAIDER¹, and RAGNAR WARNECKE² — ¹Univ. Augsburg, Inst. f. Physik, 86135 Augsburg — ²Gemeinschaftskraftwerk Schweinfurt GmbH, 97424 Schweinfurt

High temperature corrosion leads to massive problems especially in waste-to-energy-plants. At prevalent temperatures around 400°C-600°C, corrosion is mainly chlorine induced. A local release of chlorine through sulfation reaction of solid alkali chlorides is mainly responsible for the supply of chlorine at metallic components like superheaters. This reaction requires an atmosphere containing SO₂, H₂O, O₂ and releases HCl/Cl₂. Sulfates thereby generated could in combination with deposited chlorides lead to low melting eutectics in the deposit concluding in an acceleration of the corrosion process. A strategy with good prospects could be the application of additive materials in order to confine the chloride deposition. In this work the absorbing mechanism of clay minerals is examined. The additive kaolinite enables the incorporation of alkalis like Na or K. Hereby chlorine is released as gaseous HCl leading to less condensation of NaCl/KCl. Hence chlorine enrichment in the deposits can be reduced. Principles of the reaction conditions in waste-to-energy-plants, especially at the superheater tubes, are investigated and laboratory experiments regarding the encapsulation of alkalis into clay minerals, the kinetics of sulfation reactions and the corresponding chlorine attack are evaluated.

MM 49.5 Thu 11:15 BAR 205

CeMo₂B₅: a new type of arrangement of puckered boron hexagonal rings — ●SEVER FLIPO^{1,2}, MIROSLAV KOHOUT², FRIEDRICH ROTH¹, TINA WEIGEL¹, MATEJ BOBNAR², ALIM ORMECI^{1,2}, ULRICH BURKHARDT², CHRISTOPH HENNIG³, TILMANN LEISEGANG¹, DIRK CARL MEYER¹, ANDREAS LEITHE-JASPER², and ROMAN GUMENIUK^{1,2} — ¹Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Straße 23, 09596 Freiberg, Germany — ²Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden, Germany — ³ESRF, 71, Avenue des Martyrs, Grenoble, France

$REMo_2B_5$ ($RE = Ce, Pr, Nd$) and CeW_2B_5 have been synthesized. $CeMo_2B_5$ crystallizes in a new structure type with space group $Pnma$, $a = 11.0298(2)$ Å, $b = 3.12080(5)$ Å, $c = 9.9594(2)$ Å, $Z = 4$. Its structure reveals puckered [B6]-hexagonal rings, trigonal-prismatic- and empty slabs of condensed pyramids and tetrahedra. The structure can be related to the derivatives of AlB_2 and CrB prototypes. The boron atoms form a two-dimensional network of corrugated ribbons, each composed of four edge-linked [B6] rings extending infinitely along the b -axis. The Chemical bonding scenario in $CeMo_2B_5$ is dominated by the chains of [Ce₂Mo₂] clusters with multi-center bond. These clusters are connected via metallic Mo*Mo bonds and the resulting framework is stabilized by bonding interactions with the boron ribbons to which it donates electrons. $CeMo_2B_5$ is a Pauli paramagnet and electrical transport measurements, as well as the calculated density of states at the Fermi level, show $CeMo_2B_5$ to be a typical metallic system.