

## MM 30: Functional Materials III

Time: Wednesday 10:15–11:30

Location: H 0106

MM 30.1 Wed 10:15 H 0106

**Impact of alloying elements on H solubility in steels** — •ROMAN NAZAROV, TILMANN HICKEL, and JÖRG NEUGEBAUER — Max Planck Institute für Eisenforschung, Duesseldorf, Germany

Hydrogen embrittlement is a major failure mechanism in modern high-strength steels. Recent experimental studies indicate that alloying steels with selected elements largely improves their resistivity with respect to this failure mechanism. The origin of this mechanism, however, is unknown. We have therefore studied how various alloying elements affect H trapping in different steel phases. The solution enthalpies for a large set of common alloying elements in these phases have been calculated. Our results show that substitutional elements (Al, Cr, Mo, Nb, Si, Ti) energetically prefer the ferrite phase, while interstitial elements (B, C, and N) prefer austenite. Computing the interaction of these alloying elements with H we find that in the ferrite phase most of them repel an H atom from their neighborhood. In an austenitic matrix Nb and Ti bind H atoms in the first shell. Furthermore, these elements expand the Fe matrix, resulting in an increased interstitial volume and subsequent increased H solubility. In contrast, in an austenitic matrix P, Si and S repel H from their neighborhood. Based on this insight we derive a thermodynamic model which allows us to determine the solubility of H in real steels at any given temperature and H chemical potential.

MM 30.2 Wed 10:30 H 0106

**Scale Bridging Modeling of Hydrogen Embrittlement** — •DOMINIQUE KORBMACHER, CLAAS HÜTER, JOHANN VON PEZOLD, and ROBERT SPATSCHEK — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Hydrogen is known to embrittle many metals and steels, resulting in the premature failure of these materials. As a prototype of such a material we investigate nickel, which does not form hydrides under standard conditions of temperature and pressure. However, the attractive hydrogen-hydrogen interactions within the metal matrix have been shown to induce the formation of nano-hydrides in distorted regions of the lattice (crack tips or dislocations) even at only moderately enhanced hydrogen chemical potentials. We perform atomistic Monte-Carlo simulations to investigate the formation of the hydride phase as a function of the hydrogen chemical potential and use these data to parametrise a thermodynamic model with special attention to the role of elastic effects, which drastically influence the behavior in the two-phase region. The results of this analysis are then used in mesoscale simulations for the formation of hydride zones around crack tips. To this end we simulate the diffusive flux of hydrogen towards the tensile regions of a crack, and investigate the growth of the hydride zone and its steady state size depending on the stress intensity factor and the hydrogen supply. The results are in agreement with analytical scaling relations.

MM 30.3 Wed 10:45 H 0106

**Intrinsic point defects in ZnSb** — LASSE BJERG<sup>1</sup>, •GEORG K. H. MADSEN<sup>2</sup>, and BO B. IVERSEN<sup>1</sup> — <sup>1</sup>Department of Chemistry & iNANO, Aarhus University, Denmark — <sup>2</sup>Department of Atomistic Modelling and Simulation, ICAMS, Ruhr-Universität Bochum, Germany

Several efficient thermoelectric materials have been found among the

ternary Zintl antimonides. If the band structure is highly asymmetric around the band gap, the efficiency as either *n*- or *p*-type may differ significantly. The Zintl antimonides have generally been found to be *p*-type. Surprising this also holds true for the narrow band gap binary ZnSb and Zn<sub>4</sub>Sb<sub>3</sub>.

Using ab initio calculations we investigate intrinsic point defects in ZnSb as a possible origin of the *p*-type conductivity. Negatively charged Zn vacancies are found to have a low formation energy, leading to an intrinsic *p*-type behavior. We discuss this finding as a general explanation of *p*-type conductivity in Zintl antimonides and how to overcome the doping limits in these materials.

MM 30.4 Wed 11:00 H 0106

**Combined Nuclear Magnetic Resonance and x-ray diffraction study on single crystalline LiMnPO<sub>4</sub>** — •CHRISTIAN RUDISCH, SVEN PARTZSCH, JOCHEN GECK, HANS-JOACHIM GRAFE, and BERND BÜCHNER — IFW Dresden

LiMnPO<sub>4</sub> is a promising material for building the cathode of Li-ion batteries due to its high stability and large cation mobility. Yet, the mobility of the Li-ions as well as the effect of disorder on the mobility in this material is not well understood. The advantage of the use of single crystals is that the NMR linewidth is not broadened by a distribution of linewidths as in a powder sample, but can show a fine structure that could be related to different interstitial sites in the crystal. Furthermore, single crystals allow for an orientation dependent investigation of the Li-ion mobility, where certain crystal orientations are preferred by the Li-cations. We present results of a combined NMR and X-ray diffraction study which indicate a substantial degree of disorder in LiMnPO<sub>4</sub>, where the Li ions are distributed along the *b*- and *c*-axis of the crystal. The type of disorder underlines theoretical calculations which claim a possible Li-mobility in *b* direction. The impact of disorder on the Li mobility will be discussed.

MM 30.5 Wed 11:15 H 0106

**Ultra Fast and Anisotropic Diffusion of Lithium in Silicon Nanostructures** — •STEFAN WAGESREITHER, ALOIS LUGSTEIN, and EMMERICH BERTAGNOLLI — Institute for Solid State Electronics, TU-Wien, Vienna, Austria

Silicon based anodes could improve the lithium ion battery technology with a theoretical tenfold higher capacity in comparison to commercially used graphite anodes. Besides the capacity, fast charge and discharge rates and the closely associated diffusion velocity are important aspects of the battery. By improving the diffusion of lithium in silicon, an performance increase of novel silicon anodes for lithium ion batteries could be achieved. Therefore the dependency of lithium diffusion on the crystallographic directions of silicon was investigated with regard to the diffusion velocity. The lithiation of submicron silicon beams isolated on SiO<sub>2</sub> showed an anisotropic behavior with a dependency on the beam direction along the (100) plane. In silicon beams with <110> direction the lithiation was more prolonged than in <100> beams. With an approximation of the Einstein relation  $L = \sqrt{(D \cdot t)}$ , a diffusion coefficient of  $D(50^\circ\text{C}) = 3.36 \cdot 10^{-7} \text{ cm}^2/\text{s}$  was calculated which is 5 orders of magnitude higher than results for bulk silicon at the same temperature. This result is reflected in the formation of lithium silicide dendrites in the favored <110> direction after contact of lithium with a silicon thin film at room temperature.