MM 21: Hydrogen in metals IV: Special topics

Time: Tuesday 10:15–11:45 Location: TC 006

Topical Talk MM 21.1 Tue 10:15 TC 006

Hydrogenography and Metalhydride Switchable Mirrors — •Ronald Griessen — VU university, Amsterdam, The Netherlands

The discovery [1] of dramatic optical changes in metallic films loaded with hydrogen opened the way to Hydrogenography [2]. The great advantage of this new high-throughput technique is to measure optically and simultaneously on thousands of (nano)structured samples, pressure-composition isotherms, enthalpies and entropies of hydride formation. Hydrogenography provides also unique possibilities to measure reaction kinetics and catalytic activities, long-range diffusion [3], the intrinsic hydrogen permeability of alloys [4], and to optimize switchable metal-hydrides for smart windows, optic hydrogen sensors [5] and nanoantennas for active plasmonics [6].

[1] J.N. Huiberts, et al., Nature 380 (1996) 231-234; [2] R. Gremaud, et al., Advanced Materials 19 (2007)2813; [3] A. Remhof, et al., Physical Review Letters 90 (2003) 145502; [4] S. de Man et al., J. Membrane Science 444(2013)70; [5] P. Ngene et al., Adv. Funct. Mater. 2014, 24, 2374; [6] N. Strohfeldt et al., Nano Lett. 14 (2014) 1140.

MM 21.2 Tue 10:45 TC 006

A novel method for detecting hydrogen in metals at high local resolution and with ultra-high sensitivity — •Michael Rohwerder — Max-Planck-Institut für Eisenforschung GmbH

Already very low hydrogen concentrations can cause hydrogen embrittlement of high strength materials. In this presentation a novel method will be presented that allows the spatially resolved, ultra-sensitive measurements of hydrogen in steels and other alloys as well as its uptake into and permeation through them [1-4]. Several examples demonstrating the capabilities of this novel, Kelvin probe based technique will be presented. Finally, an example will be given demonstrating the role of localized hydrogen enrichments for hydrogen embrittlement of TWIP steels.

References:

[1] C. Senöz, S. Evers, M. Stratmann and M. Rohwerder, Electrochem. Commun. 13 (2012)1542

[2] S. Evers, M. Rohwerder, Electrochem. Commun. 24 (2012) 85

[3] S. Evers, S. Ceylan, M. Rohwerder, Science and Technology of Advanced Materials 14 (2013) 014201

[4]S. Evers, C. Senöz, M. Electrochimica Acta 110 (2013) 534

MM 21.3 Tue 11:00 TC 006

Thermal desorption spectra from 3D materials — •Thomas Schablitzki, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Deutschland

Temperature programmed desorption (TPD) is frequently used in surface science to characterise adsorption sites and reactions on surfaces. It can also be applied to bulk materials to study the trapping of solute atoms at point and extended defects, such as vacancies, grain boundaries or dislocations. Using a kinetic Monte Carlo (kMC) approach to simulate TPD spectra for surfaces has provided valuable information for the interpretation of the different contributions to the spectra.

Here we simulate TPD spectra for bulk systems. The kMC Model consists of a 3D lattice with a surface and we include the effect of bulk diffusion on the TPD spectra. The effect of various defects on diffusion and the resulting desorption spectra are analysed.

MM 21.4 Tue 11:15 TC 006

Chemical Trends Of Interstitial Solubility In Transition Metals: DFT Driven High-Throughput Databases — •Ugur Aydin, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Deutschland

We present insights for chemical trends of the solubility of interstitial elements H, He, B, C, N, O, F, Ne in 3d, 4d, 5d transition metals obtained with High-Throughput DFT calculations. The parallel generation of the bulk-interstitial systems and their systematic investigation with an in-house developed workbench, called *pyCMW*, allowed us to classify the elastic and chemical mechanisms governing the solution enthalpy of the interstitials mentioned above. The introduction of a correlation coefficient $r_{xy} \in [0, 1]$ between the bulk modulus B_0 and the solution enthalpy ΔH gives a qualitative insight for both mechanisms. While for non-reactant interstitial elements, the noble gases He and Ne, $r_{xy} = 0.97$ indicates a very high elastic but a very low chemical impact on ΔH, interstitial hydrogen shows with $r_{xy} = 0.03$ (very high chemical but very low elastic contribution) an inverse behavior. In a similar way all interstitial elements can be ordered according to the chemical and elastic impact on ΔH.

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