MM 11: Interfaces III

Time: Monday 14:45–15:45 Location: H6

MM 11.1 Mon 14:45 H6

Carbide precipitation at a grain boundary in molybdenum - an ab-initio DFT study — •Rebecca Janisch[1] and Christian Elsässer[2] — [1]Universität Erlangen-Nürnberg, Institut für Werkstoffwissenschaften (WWI), Martensstr. 5, 91058 Erlangen, Germany — [2]Fraunhofer-Institut für Werkstoffmechanik, Wöhlerstr. 11, 79108 Freiburg, Germany

Atomic-scale stages of the growth of an interfacial precipitate film of tetragonal molybdenum carbide at a Σ5 (310) [001] symmetrical tilt grain boundary in molybdenum were investigated by means of atomistic supercell calculations on the basis of ab-initio density functional theory (DFT). In this presentation, the structural development of the precipitate with increasing carbon concentration is analysed. The structurally optimised atomistic model for the fully developed precipitate is compared to experimental high-resolution images from transmission electron microscopy, and it allows to clarify some ambiguous features therein. An atomic-scale twinning mechanism in the MoC precipitate is proposed. Finally, the influence of the carbon concentration on the stability of the metal-carbide interface with respect to cleavage is discussed.

MM 11.2 Mon 15:00 H6

The role of crystallography in topotaxial first-phase selection — •Andriy Lotnyk, Stephan Senz, and Dietrich Hesse — Max Planck Institute of Microstructure Physics

The role of crystallography in topotaxial first phase formation in the MgO-TiO_2 system is studied. The question which phase forms first in a thin-film solid state reaction, if the corresponding phase diagram permits the formation of several phases, is of considerable scientific and technological significance. Correspondingly, a number of models have been put forward, including kinetic, thermodynamic, and nucleation-related models. In the present work, vapor-solid reactions between MgO (vapor) and TiO_2 (rutile) single crystals with different surface orientations were performed. The crystallographic relations between the product phases and the TiO_2 substrates were studied by X-ray diffractometry and transmission electron microscopy. A topotaxial formation of $MgTiO_3$ on the rutile crystals was found. Previous results on vapor-solid reactions of TiO_2 (vapor) with MgO substrates showed the topotaxial formation of Mg_2TiO_4. We conclude that in the MgO-TiO_2 system, in case of a topotaxial solid state reaction, the phase forming first depends on the crystallography of the substrate serving as reactant. Thus, crystallography obviously can play an important role in the determination of the first growing phase in topotaxial solid-state reactions.

MM 11.3 Mon 15:15 H6

Al-Al Compound Casting — •Konrad Papis, Peter Uggowitzer, and Jörg Löffler — ETH Zurich, Laboratory of Metal Physics and Technology, Zurich, Switzerland

'Compound casting' is a process where a melt is cast onto or around a solid metallic 'insert'. It is the realization of a simple joining procedure for light metals aimed at weight-saving. Difficulties inherent in joining aluminium are its natural oxide layer and the formation of intermetallic phases. In this project, both the solid substrate and the melt used are aluminium alloys containing various alloying elements (Cu, Si, Zn in the melt, Mg in the substrate). Compounds with flawless interfaces (no contraction defects, no oxides) were successfully produced by replacing the oxide layer with a zinc layer. This was accomplished by pickling the substrate in a solution containing zincate ions, implying a redox reaction by which zinc is deposited in its metallic form. The composition and mechanical properties of the compounds' interfacial regions were investigated by SEM/EDX and microhardness measurements following the 'compound casting' process and successive heat treatments. DICTRA calculations were carried out to simulate the diffusion processes at the interface. The results from the mechanical characterization were compared to the simulations, the conclusion being that diffusion of alloying elements led to precipitation hardening of the compound.

MM 11.4 Mon 15:30 H6

Investigation of Fe/MgO interfaces by Atom Probe Tomography (APT) — •Alexander Mackel, Talaat Al-Kassab, and Reiner Kirchheim — Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077 Göttingen

Modern magnetic storage devices such as Magneto-resistive RAM (MRAM) devices are generally built up from a stack of thin layers, in which one of these layers is an oxide-barrier. The effect of Tunnelling Magneto-Resistance (TMR), governing the function of these devices, is strongly dependent on the electron transmission, in particular, at the Oxide/Metal interface. Therefore, it becomes important to characterize these interfaces on the nano-scale concerning their geometrical and chemical roughness. With this objective, we investigated the stacking of an ideal Fe/MgO/Fe sandwich type by means of APT.

The layers were prepared by ion beam sputtering on tungsten substrate-tips of 30 to 50nm radius of curvature as well as on Si-posts with a planar surface. Using a Focused Ion Beam, these posts were formed into a needle-like shaped tip to enable APT investigation.

The model system has been analyzed successfully for barrier thicknesses smaller than 2nm. So far, we found a FeO-peak in the time-of-flight mass spectrum of the interface indicating that Fe is partly oxidized already in the as-prepared state. The origin and presence of the FeO will be discussed as well as a comparison between the results obtained from both types of samples.

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