MM 6: Diffusion and Point Defects II

Time: Monday 11:30–12:30 Location: H6

MM 6.1 Mon 11:30 H6

Study of ^{44}Ti grain boundary self diffusion in thin nanocrystalline TiO_2 films — •Petr Straumal[1,2], Ata Myatiev[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Muenster, Germany — [2]National University of Science and Technology "MISIS", Leninsky Prospect 4, 119049 Moscow, Russia

Titanium dioxide is known for its photo-catalytic properties and enhanced corrosion resistance in aqueous environments. For catalytic applications it is helpful to dope the TiO_2 with metal dopants which can move the absorption edge of TiO_2 from the UV to the blue region of the visible spectrum. Also the electrical conductivity of non-stoichiometric TiO2 is proportional to the concentration of oxygen vacancies. The grain boundary diffusion plays a significant role in both processes. Numerous works are dedicated to the diffusion of various dopants like niobium or chromium in TiO_2 but so far, none studied the self diffusion of titanium. The grain boundary self diffusion in thin nanocrystalline TiO_2 films is investigated. The oxide films are produced using a novel deposition method from metal-organic precursors at relatively low (400-500°C) temperatures. The diffusion was measured by means of the radiotracer technique applying the ^{44}Ti isotope and utilizing ion beam sputtering for sectioning. In addition, the microstructure was investigated using TEM. The results are discussed with respect of the relationship between grain boundary self diffusion and the synthesis pathway and resulting microstructure of the nanoscale functional oxide films. Support by DAAD is gratefully acknowledged.

MM 6.2 Mon 11:45 H6

Self-diffusion of Ti and ultra fast solute diffusion of Co in annealed and severely deformed α-Ti — •Jochen Fiebig[1], Sergiy Divinski[1], Yuri Estrin[2], and Gerhard Wilde[1] — [1]Institute of Material Physics, Westfälische Wilhelms University, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Monash University, Claytoon, Victoria, Australia

Severely deformed materials attain nowadays a growing technological interest due to their advanced properties and property combination. In the present study we compared the diffusion properties, especially grain boundary diffusion, of coarse-grained and ultra fine-grained α-Ti. The severe deformation was performed by equal channel angular pressing. The radiotracer method was used in combination with the parallel sectioning technique. With this method we studied the self-diffusion of ^{44}Ti and the impurity diffusion of the so called 'fast diffuser' ^{57}Co in α-Ti before and after severe plastic deformation. For ^{57}Co ultra-fast diffusion rate along the grain boundaries in annealed α-Ti was observed which is significantly decreased after severe plastic deformation. The diffusion data is discussed with respect to the possible existence of 'non-equilibrium' grain boundaries in severely deformed materials. Support by DFG is gratefully acknowledged.

MM 6.3 Mon 12:00 H6

Untersuchung von Korngrenzen in Kupfer mithilfe eines Feinfokus-Positronen-Strahles — •Reinhard Sottong, Patrick Eich, Matz Haaks und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn

Die Positronen-Annihilations-Spektroskopie (PAS) ist eine renommierte Methode zur Untersuchung von Kristalldefekten. Die Positronen dienen hierbei als Sondenteilchen, mit denen einzelne Fehlstellen beobachtbar sind.

Durch Glühen von OFC-Kupfer bei 1000°C und langsames Abkühlen auf Raumtemperatur wurden in einer Probe Körner mit einer Größe von 40 μm mal 100 μm erzeugt. Unter mechanischer Beanspruchung stellen die Korngrenzen Hindernisse für das Gleiten von Versetzungen dar, wodurch es hier zu einem Stapeln der Versetzungen kommt.

Mit der Bonner Positronen-Mikrosonde (BPM) wurde die Fehlstellendichte an einem Korn mit einer Ortsauflösung von 1 μm sowohl im unverformten Zustand als auch nach plastischer Deformation untersucht. Der Vergleich dieser Messergebnisse zeigt eine Erhöhung der Fehlstellendichte an den Korngrenzen. Positronen als Fehlstellensonden mit hoher Ortsauflösung sind ein einfaches Verfahren, um z.B. Versetzungsaufstau an Hindernissen bei schwacher Verformung zu beobachten.

MM 6.4 Mon 12:15 H6

Ultra-slow lithium diffusion in Li_3NbO_4 probed by ^{7} Li stimulated echo NMR spectroscopy — •Benjamin Ruprecht and Paul Heitjans — Institut für Physikalische Chemie und Elektrochemie, Leibniz Universität Hannover, D-30167 Hannover

Currently, a variety of fast Li conductors attract much attention due to possible future applications in batteries. In contrast, apart from fundamental aspects, for other applications such as breeder materials for fusion reactors materials with exceptionally slow Li transport are needed. We present studies on the ultra-slow Li transport in the model system Li_3NbO_4 (cubic, space group $I\text{-}43m$) by ^{7}Li Spin-Alignment Echo Nuclear Magnetic Resonance (SAE NMR) spectroscopy [1]. NMR spectroscopy allows one to probe ionic transport on a microscopic scale. In Li_3NbO_4 the Li ions reside in different electrical field gradients at the nuclear sites giving rise to different quadrupolar precession frequencies ω_Q. Diffusion induced changes of ω_Q during the mixing time t_m of the pulse sequence used lead to a decay of the stimulated echo observed. By recording the t_m dependence of the echo amplitude the SAE NMR experiment yields two-time single-particle correlation functions and gives direct access to correlation rates τ_c^{-1} which may be identified with Li jump rates [2]. In the case of Li_3NbO_4 ultra-slow lithium jumps in the regime $1..10^4\,s^{-1}$ (373..553 K) were found showing that Li_3NbO_4 is indeed a very poor lithium ion conductor.

[1] R. Böhmer, K. R. Jeffrey, M. Vogel, Prog. Nucl. Magn. Reson. Spectrosc. 50 (2007) 87

[2] M. Wilkening, P. Heitjans, Solid State Ion. 177 (2006) 3031.