MM 19: Transport

Time: Tuesday 14:00–15:30 Location: IFW D

MM 19.1 Tue 14:00 IFW D

Transport and magnetic properties of non-stochiometric FeSi — Monika Kotzian, Tommy Reimann, Dirk Schulze Grachtrup, Stefan Süllow, and •Dirk Menzel — Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany

Although the narrow-gap semiconductor FeSi has a non-magnetic ground state, it shows a residual Curie-like susceptibility at low temperature. Whereas this Curie-tail was generally attributed to a surplus of Fe^{3+}, magnetic measurements imply that the residual susceptibility of samples with a slight Fe deficit is larger compared to samples with Fe excess. The transport properties of off-stochiometric tri-arc Czochralski-grown FeSi crystals have been investigated. The temperature dependence of the conductivity suggests that Anderson-localized states which stem from structural disorder carry the residual magnetic moment. Magnetoresistance measurements, which give some indications for a weakly localized system, support this interpretation. In addition, within an impurity model they show that the number of such localized states in the off-stochiometric samples is larger for Fe deficit than for Fe excess. Annealing experiments reveal that the off-stochiometry has a larger influence on the magnetic and transport properties than the presence of crystalline imperfections.

MM 19.2 Tue 14:15 IFW D

Fast grain boundary self-diffusion in ultrafine grained Ag produced by equal channel angular pressing — •Jochen Michael Fiebig[1], Werner Skrotzki[2], Sergiy V. Divinski[1], Martin Peterlechner[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische Wilhelms Universität, 48149 Münster — [2]Institut für Strukturphysik, Technische Universität Dresden

We performed a systematic study of grain boundary self-diffusion in ultrafine grained silver produced by equal channel angular pressing (ECAP) using samples deformed up to 3 passes according to route A. The resulting ultra-fine grained microstructure was studied by transmission electron microscopy and electron backscatter diffraction. The radiotracer method (^{110m}Ag-tracer solution) in combination with parallel sectioning by microtome slicing was used to obtain the diffusion properties. The activity of each section was counted by a high-purity Ge detector. The grain boundary diffusion was measured depending on the deformation state and the resulting profiles unambiguously revealed the existence of grain boundaries with enhanced excess energy density, i.e. so-called *non-equilibrium* grain boundaries. Percolating porosity, as already observed for Cu and Cu-alloys produced by ECAP also exists in ECAP-Ag. Applying Borisov's formalism the excess energy of non-equilibrium grain boundaries was determined. The energy of general high-angle grain boundaries was measured to be about 0.5 J/m^2. The grain boundary energy of non-equilibrium grain boundaries is about 10% to 15% higher.

MM 19.3 Tue 14:30 IFW D

Grain Boundary Diffusion in Ultra Fine Grained Copper Produced by High Pressure Torsion — •Matthias Wegner[1], Jörn Leuthold[1], Martin Peterlechner[1], Daria Setman[2], Michael Zehetbauer[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, D-48149 Münster, Germany — [2]Physics of Nanostructured Materials, University of Vienna, A-1090 Wien, Austria

Short-circuit diffusion paths in Ultra Fine Grained copper produced by High Pressure Torsion (HPT) are investigated by the radiotracer method. *Ultra fast* diffusion in addition to conventional grain boundary diffusion is observed. This feature might be related to the existence of so called Non Equilibrium Grain Boundaries (NEGBs) acting as ultra fast diffusion paths. According to the existing models of grain refinement by severe plastic deformation (as e.g. HPT), the abundance of lattice dislocations created during the severe straining serves to modify the grain boundary structure of high angle grain boundaries such that NEGBs with enhanced excess free energy densities are created. The kinetics and structural properties of NEGBs are thoroughly investigated. Furthermore, a network of percolating porosity introduced during the HPT process is observed. This unexpected feature is investigated utilizing the radiotracer technique. A strong dependence of the effective diffusivity and the volume fraction of the porosity on the applied quasi-hydrostatic pressure during HPT is elucidated.

MM 19.4 Tue 14:45 IFW D

Diffusion in a Cu bicrystal with near Σ5 grain boundary — •Henning Edelhoff[1], Sergej Prokofjev[2], Sergij Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Institute of Solid State Physics, Chernogolovka, Moscow region, Russia

For the overall understanding of kinetic processes along grain boundaries of polycrystalline and nanocrystalline materials it is essential to understand the processes in a single, well defined grain boundary. In this work, for the first time, the grain boundary diffusion of a solute is measured in a single grain boundary in the C kinetics regime according to the common Harrison classification. The radiotracer technique in combination with parallel sectioning by microtome is used to determine ^{110m}Ag diffusion rates in Cu Σ5 (310) [001] bicrystal along and perpendicular to the <001> misorientation axis under formal conditions of the B-type and C-type regime.

These studies provided in the B-type regime the values of the triple product $P = s \cdot d \cdot D_{gb}$ of the segregation coefficient s, the effective (diffusional) grain boundary width d and the grain boundary diffusion coefficient D_{gb}, with the latter being directly determined in the C-type regime. A moderate but measurable anisotropy of the grain boundary diffusion is established. The anisotropy of the product $s \cdot d$, which could be related to a heterogeneous segregation of Ag in the grain boundary, is estimated.

MM 19.5 Tue 15:00 IFW D

Recent advances in grain boundary diffusion studies — •Sergiy Divinski — Institute of Materials Physics, University of Münster

A short overview of a recent progress in experimental investigation of grain boundary diffusion and segregation phenomena is presented. The talk is focused on solute diffusion in bi- and tri-crystals. Using the radiotracer technique in combination with serial sectioning and applying precisely characterized bicrystals, the grain boundary diffusion was for the first time measured at low temperatures under the C kinetic conditions [1] after common Harrison's classification. The anisotropy of the grain boundary diffusion coefficient, D_{gb}, and that of the triple product P, $P = s \cdot \delta \cdot D_{gb}$, was measured for Ag diffusion in Cu near Σ5 grain boundary. The data are discussed in relation to the grain boundary structure.
The first measurements of Ag diffusion along a triple line in tri-crystal [2] are presented and discussed with respect to the triple line energy.
1. H. Edelhoff, S.I. Prokofjev, S.V. Divinski, Scr. Mater. (2010) doi: 10.1016 j.scriptamat.2010.10.032
2. S.V. Divinski, H. Edelhoff, G. Gottstein, L.S. Shvindlerman, B. Zhao, to be published.

MM 19.6 Tue 15:15 IFW D

Study of 44Ti grain boundary self-diffusion in thin nanocrystalline TiO2 films — •Petr Straumal[1,2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Universität Münster, D-48149 Muenster, Germany — [2]National University of Science and Technology "MISIS", 119049 Moscow, Russia

Titanium dioxide is known for its photo-catalytic properties and enhanced corrosion resistance in aqueous environments. Due to these properties TiO2 is very attractive material for light-induced self-cleaning glass, water-cleaning and producing hydrogen from water applications. Numerous works are dedicated to the diffusion of various dopants like niobium or chromium in TiO2 but so far, none studied the self-diffusion of titanium in nanocrystalline TiO2. The grain boundary self-diffusion in thin nanocrystalline TiO2 films is investigated. The oxide films are produced using a novel deposition method from metal-organic precursors at relatively low (400-500°C) temperatures. A relaxation annealing at 800°C was performed. The diffusion was measured in temperature interval between 200°C and 600°C by means of the radiotracer technique applying the 44Ti isotope and utilizing ion beam sputtering for sectioning. The diffusion was measured at different oxygen pressures. In addition, the microstructure and its possible evaluation during diffusion annealing was investigated using TEM. The results are discussed with respect of the relationship be-

tween grain boundary self-diffusion and the synthesis pathway, the oxygen pressure and resulting microstructure of the nanoscale functional oxide films.