

MM 32: Diffusion and point defects I

Time: Thursday 10:15–11:15

Location: H6

MM 32.1 Thu 10:15 H6

Diffusion of Hydrogen in Amorphous Ceramics of the System Si-B-C-N — ●WOLFGANG GRUBER, GÜNTER BORCHARDT, and HARALD SCHMIDT — TU Clausthal, Institut für Metallurgie, Thermochemie und Mikrokinetik - AG Materialphysik

Non-oxide ceramics of the system Si-B-C-N have potential applications as high temperature structure materials, surface coatings and dopable semiconductors. Materials produced from polymeric precursors which are transformed into amorphous covalent ceramics by solid state thermolysis are separated in a silicon rich phase and a carbon rich phase. Diffusion of hydrogen plays an important role in the investigation of the mobility and the kind of defects in the amorphous state. Therefore we measured the diffusivities of hydrogen in amorphous ceramics of the system Si-B-C-N with different compositions. For the diffusion measurements we used deuterium as a tracer which was introduced into the samples via isotope exchange from the gas phase. Depth profiling was done with secondary ion mass spectrometry (SIMS). Depending on the composition the diffusion path for hydrogen is the carbon rich phase or the silicon rich phase. A direct interstitial diffusion mechanism accounts for the diffusion of hydrogen in the carbon rich phase and a trap limited diffusion mechanism accounts for the diffusion of hydrogen in the silicon rich phase.

MM 32.2 Thu 10:30 H6

Diffusion-induced recrystallization in thin metal films — ●DIETMAR BAITHER, BRITTA KRUSE, TAE HONG KIM, and GUIDO SCHMITZ — Westfälische Wilhelms-Universität, Institut für Materialphysik, Wilhelm-Klemm-Strasse 10, D-48159 Münster

Diffusion-induced recrystallization (DIR) was investigated in AuCu and AgPd double layers. The layers were prepared by sputter deposition on glass substrates. In spite of large lattice mismatch of 13.0 % and 5.1 % for the AuCu and AgPd system, respectively, the thin layers grow semi-coherently with (111) texture.

After heat treatment at 708 K or 723 K, various additional intensity maxima occur in the XRD spectra in dependence on the duration of heating. Simulated XRD spectra point out that these maxima cannot be explained by volume diffusion, even if a concentration-dependant diffusion coefficient is supposed. Instead, the existence of new grains with a preferred composition is favoured. Such newly formed grains were found in TEM micrographs of both systems. EDX measurements confirm the transformation of the planar interface into a granular region of distinct composition.

The evolution of the microstructure and the growth of grains with preferred discrete compositions will be described by a thermodynamical model, which considers the elastic stress and its relaxation during recrystallization.

MM 32.3 Thu 10:45 H6

Grain boundary phase transitions in Cu–Bi alloys studied

by radiotracer grain boundary diffusion measurements —

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Bismuth addition to copper is known to cause a catastrophic embrittlement of the material. Moreover, strong Bi segregation at copper grain boundaries may result in the formation of a liquid-like layer even in the Cu-rich single-phase region of the corresponding bulk phase diagram [1]. Since the grain boundary diffusion depends very sensitively on the boundary structure, the rate of grain boundary diffusion can serve as a unique probe of phase transitions occurring when alloying Cu with Bi.

In the present investigation, grain boundary diffusion and segregation of Bi in polycrystalline Cu–Bi alloys are investigated by the radiotracer serial sectioning technique using the ²⁰⁷Bi isotope. An observed non-Arrhenius temperature dependence of grain boundary diffusion of Bi is discussed in relation to the prewetting phase transition at grain boundaries in the Cu–Bi system.

1. S.V. Divinski, M. Lohmann, Chr. Herzig, et al. Phys. Rev. B. 71 (2005) 104.

MM 32.4 Thu 11:00 H6

Ungewöhnliche Diffusion von Ag und Cu in CdTe —

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Normale Diffusion äußert sich in einer von der Quelle ausgehenden monotonen Abnahme des Konzentrationsprofils. Im Gegensatz dazu zeigen die Diffusionsprofile von Ag und Cu in den II-VI Halbleitern CdTe, ZnTe und CdZnTe ein völlig anderes Verhalten, wenn die Diffusion unter einem externen Dampfdruck der Metallkomponente durchgeführt wird [1]. So wird in CdTe nach Implantation von ¹¹¹Ag oder ⁶⁷Cu und Tempern bei 825 K ein Profil beobachtet, das symmetrisch im Querschnitt des 800 μm dicken Kristall liegt, wobei die ¹¹¹Ag Konzentration im Zentrum gegenüber den Randschichten fast stufenartig zunimmt und dort 20-fach erhöht ist. Wird hingegen das Diffusionstempern unter externem Te Druck durchgeführt, tritt in den Randbereichen des CdTe Kristalls eine gegenüber dem Kristallinneren stark erhöhte Ag Konzentration auf. Ein quantitatives Modell wird vorgestellt. Dieses Modell berücksichtigt den Einfluss des externen Dampfdrucks während des Temperns und damit die durch die Diffusion intrinsischer Defekte verursachte Änderung der Stöchiometrieabweichung des CdTe Kristalls. Außerdem wird die elektrische Drift geladener Defekte im internen elektrischen Feld, das durch die Konzentrationsprofile der geladenen Defekte verursacht wird, berücksichtigt.

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[1] H.Wolf *et al.*, Phys. Rev. Lett. 94 (2005) 125901.