MM 20: Transport & Diffusion I

Time: Tuesday 10:15–11:30 Location: H26

MM 20.1 Tue 10:15 H26

Temperature dependent structure transition of a Σ17 (410) grain boundary in copper investigated by the radiotracer technique — •Henning Edelhoff[1], Harald Rösner[1], Sergei Prokofjev[2], Gerhard Wilde[1], and Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Institute of Solid State Physics, Chernogolovka, Russia

Due to the increasing amount of grain boundaries in fine- and ultra fine-grained materials, the effect of interfaces on materials properties is of great importance. Still the fundamental understanding of grain boundaries and their energy, structure and kinetics as a function of temperature and solute segregation is incomplete. A promising method to gain the information about kinetics and structure is to use the radiotracer technique with individual well characterized grain boundaries.

In the previous work on Ag diffusion in a Cu grain boundary of "near Σ5 (310)"-type, a structural transition of the grain boundary was observed at approximately 850 K, which also appears in MD simulations.

To take a closer look on possible structure transitions within interfaces, a Σ17 tilt grain boundary is investigated in the temperature range from 714 K to 952 K. The grain boundary diffusion of 110m-Ag in a Cu Σ17(410) bi-crystal is measured along the misorientation axis and the results are interpreted on the basis of TEM and MD simulation.

MM 20.2 Tue 10:30 H26

Formation and growth of Cu3Si studied by SNMS — •Zoltán Balogh[1], Mohammed Ibrahim[1], Guido Schmitz[1], Bence Parditka[2], and Zoltán Erdélyi[2] — [1]Westfälische Wilhelms Universität-Münster Wilhelm Klemm Straße 10, Münster, D-48149 (Germany) — [2]University of Debrecen PO Box. 2, Debrecen, H-4010 (Hungary)

Metal induced crystallization is one of the methods to reduce the crystallization temperature of amorphous Si films [1]. This can happen either by the bond weakening effect of eutectic forming materials or by assistance of metal-silicide template. Metal-Si solid state reactions also represent some of the very few examples in which a linear kinetics in the formation of an intermetallic layer is observed [2,3].

We investigated the formation and the subsequent growth of the Cu/Si reaction layer in sputter deposited thin films. Bilayers comprising 45 nm Cu on 120 nm a-Si were deposited upon Si <100> substrates and annealed at 135 °C under high vacuum conditions. XRD revealed that Cu3Si does grow as a result of the annealing. By SNMS and XPS investigations we found that (i) the Cu3Si layer is not present in the as-deposited layer, (ii) a 20 nm thick layer is quickly formed after very short annealing and that (iii) further growth appears linearly with significantly slower rate of 1 nm/h.

[1] Z. Wang et al., Adv. Eng. Mater., 11 (2009) 131.
[2] F.M. d'Heurle and P. Gas, J. Mater. Res., 1 (1986) 205.
[3] F. Nemouchi et al., Appl. Phys. Lett., 86 (2004) 041903.

MM 20.3 Tue 10:45 H26

Growth kinetics and interface structure of copper silicides studied by atom probe tomography — •Mohammed Ibrahim, Zoltán Balogh, Patrick Stender, Mohammed Reda Chellali, and Guido Schmitz — Westfälische Wilhelms Universität-Münster Wilhelm Klemm Straße 10, Münster, D-48149 (Germany)

The production of crystalline Si films is important for numerous applications. In contact with some silicide forming components, the crystallization temperature of amorphous Si is significantly reduced [1]. Si deposited on Cu is also considered as a possible anode for high capacity Li-ion batteries. Solid state reaction between the Si and the Cu current collector results in the formation of copper-silicides [2]. Gaining information on the kinetics of this reaction is thus desired for many applications.

We investigated the early phases of the growth of Cu-silicides by laser assisted APT [3]. Cu and Si have been deposited upon field developed tungsten (W) tips. We found that an intermixed zone is already formed during the deposition. Its thickness strongly depends on the stacking order. The transition zone is broad in the case of Cu on Si and much sharper for Si on Cu. After annealing at 130 °C (from 30 min to 4 hours) we observe formation of a Cu3Si layer with few tens of nm thickness. Remarkably Si segregates to the free surface and to the Cu/Cu3Si interface.

[1] Z. Wang et al., Adv. Eng. Mater., 11 (2009) 131.
[2] H. Chen et al., J. Power Sources, 196 (2011) 6657.
[3] R. Schlesiger et al., Rev. Sci. Instrum., 81 (2010) 043703.

MM 20.4 Tue 11:00 H26

Solute diffusion along interfaces in nanocrystalline copper — •Matthias Wegner[1], Jörn Leuthold[1], Martin Peterlechner[1], Xiaoyan Song[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]University of Münster, Institute of Materials Physics, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — [2]Beijing University of Technology, 100124 Beijing, China

Diffusion of solutes along interfaces in nanocrystalline copper with grain sizes of about 40 and 50 nm produced by Spark Plasma Sintering (SPS) is investigated by means of the radiotracer technique. The small grain size in addition to the good thermal stability of SPS Cu yields a unique opportunity to measure radiotracer diffusion in a nanocrystalline material without complicating effects like grain boundary motion, grain growth or recrystallization. Diffusion measurements were done within the temperature regime of 435 K up to 470 K. The results are discussed with respect to a potential influence of triple junction diffusion on the measured diffusion profiles. Possible mechanisms which may be responsible for stabilizing the microstructure of the nanocrystalline copper up to temperatures of ~ 1/3 of the melting temperature are elucidated. Furthermore the amount of porosity and its effect on the measurements is discussed. As a main result, the absence of a size dependence of the specific grain boundary diffusion rate is observed.

MM 20.5 Tue 11:15 H26

Experiments on the Investigation of Self-Diffusion in Amorphous Silicon — •Florian Strauss[1], Harald Schmidt[1], Jochen Stahn[2], and Thomas Geue[2] — [1]TU Clausthal, AG Mikrokinetik, Institut für Metallurgie, Deutschland — [2]Paul Scherrer Institut, Villigen, Schweiz

A key task in material science is the investigation of self-diffusion in solids in order to characterize kinetic processes and to identify point defects and process relevant activation energies. In spite of its technological importance, e.g. in photovoltaic cells, there are no experimental data in current literature on the self-diffusion in amorphous silicon (a-Si). This is mainly due to a combination of the expected low diffusivities and the intrinsic metastability of a-Si in the accessible time and temperature range. In order to determine self-diffusivities $^{29}Si/^{28}Si$ isotope multilayers are prepared by ion-beam sputtering. Afterwards those samples are thermally treated in Ar atmosphere at different temperatures below the crystallization limit in order to induce diffusion. The isotope multilayers are amorphous and chemically homogeneous (as shown by TEM and XRD) but isotope-modulated. Consequently diffusion can be measured by time-of-flight neutron reflectometry, a method capable of determining extremely small diffusion lengths in the order of 1 nm and below [1,2]. First results point to an onset of diffusion at about 350 °C. The influence of O impurities on structure and diffusion is discussed.

[1] H. Schmidt et al.; Acta Mater. 56 (2008), 464
[2] E. Hüger et al., Appl. Phys. Lett. 93 (2008), 162104