MM 16: Diffusion and Point Defects I

Time: Tuesday 11:30–12:30 Location: IFW B

MM 16.1 Tue 11:30 IFW B

Diffusion and Crystallization in Magnetron Sputtered SiC Films — •Wolfgang Gruber and Harald Schmidt — TU Clausthal, Institut für Metallurgie, AG Materialphysik

Thin films of amorphous and polycrystalline SiC have a great potential for applications in various branches of technology. For a tailored production of polycrystalline films a understanding of nucleation and growth mechanisms which determine the microstructure are necessary. X-ray diffractometry (XRD) and transmission electron microscopy (TEM) studies on r.f. co-sputtered SiC films yielded a strong dependence of the crystallization rates on the substrate. For single crystalline silicon as a substrate an activation energy of about 4 eV is found for the rate of crystallization. If glassy carbon is used as a substrate the corresponding activation energy is about 9 eV. For a closer investigation of this phenomenon, in this study we investigated films deposited on different substrates with different thickness (100 nm to 1000 nm) and variable composition SiCx. Since self-diffusion plays an important role for crystallization we measured the diffusivities of the constituting elements using isotope enriched heterostructures and secondary ion mass spectrometry (SIMS). Based on the experimental results a model for crystallization kinetics is discussed.

MM 16.2 Tue 11:45 IFW B

Atom Jumps Studied by Coherent Synchrotron Radiation — •Gero Vogl[1], Michael Leitner[1], Bastian Pfau[2], Bogdan Sepiol[1], and Lorenz-Mathias Stadler[1] — [1]Fakultät für Physik der Universität Wien, Austria — [2]BESSY, Berlin, Germany

Measuring the atomic diffusion jump is a fundamental problem in solid state physics. Up to now only measurements involving a limited number of isotopes and in a very limited temperature range were feasible due to the limitations of methods such as quasi-elastic neutron scattering, quasi-elastic Mössbauer spectroscopy or nuclear magnetic resonance.

X-ray photon correlation spectroscopy has the potential to overcome these constraints. We present the first successful implementation of this new technique. We deduce the atomic jump model from the q-dependent relaxation times of diffuse scattering measured at the ESRF and give the activation energy of Au diffusion in CuAu. We predict that the new sources with increased brilliance and high coherence like PETRA or the XFEL will enable determination of the atomic diffusion jump in condensed matter over a wide range.

MM 16.3 Tue 12:00 IFW B

Self-diffusion in Germanium at Low Temperatures — •Erwin Hüger[1], Ursula Titze[2], Dieter Lott[2], Hartmut Bracht[3], Dominique Bougeard[4], Eugene E. Haller[5], and Harald Schmidt[1] — [1]TU Clausthal, Germany — [2]GKSS Forschungszentrum Geesthacht, Germany — [3]Universität Münster, Germany — [4]TU München, Germany — [5]University of California at Berkeley, USA

Self-diffusion in intrinsic single crystalline germanium was investigated between 429 and 596 °C using $^{70}Ge/^{nat}Ge$ isotope multilayers. The diffusivities were determined by neutron reflectometry from the decay of the first and third order Bragg peak. At high temperatures the diffusivities are in excellent agreement with literature data obtained by ion beam sputtering techniques, while considerably smaller diffusion lengths between 0.6 and 4.1 nm were measured. At lower temperatures the accessible range of diffusivities could be expanded to values $D < 1 \times 10^{-25}$ m^2s^{-1} which is three orders of magnitude lower than the values measured by sputtering techniques. Taking into account available data on Ge self-diffusion, the temperature dependence is accurately described over nine orders of magnitude by a single Arrhenius equation. An activation enthalpy of diffusion of (3.13 ± 0.03) eV and a pre-exponential factor of 2.54×10^{-3} m^2s^{-1} for temperatures between 429 and 904 °C are obtained. Single vacancies are considered to prevail self-diffusion in Ge over the whole temperature range.

MM 16.4 Tue 12:15 IFW B

Defect structures in CaF_2 for optical applications — •Stephan Rix[1,2], Marisa Aigner[1], Claudia Felser[2], Martin Letz[1], Ute Natura[3], and Lutz Parthier[3] — [1]Schott AG, Mainz — [2]Johannes Gutenberg-Universität, Mainz — [3]Schott Lithotec, Jena

Single crystal calcium fluoride (CaF_2) is an important lens material for deep-ultraviolet optics used in microlithographic structuring of semiconductors. High radiation densities require an extreme laser-stability of the material. The quality of the material strongly depends on a high purity level. For long exposure times the optical quality of CaF_2 is affected by radiation-induced defect structures, namely F- and H-centers. The migration and agglomeration of these defect structures play an important role in understanding laser-damage processes on a microscopic level. We use ab-initio methods to investigate the stabilization of laser-induced defects by agglomeration or impurities. As stabilization processes involve defect migration, we also focus on diffusion properties of defects. We present a method for the calculation of diffusion barriers, which shows good agreement with experimental results for the F-center with well localized electronic wave functions.