FM 7: Crystal Defects and Real Structure Physics in Diamond and Functional Materials I

chair: Theo Scherer (Karlsruhe Institute of Technoloy, DE)

Time: Tuesday 9:30–11:45 Location: BEY/0E40

FM 7.1 Tue 9:30 BEY/0E40

Fluorescence lifetime measurements of NV- and NV0 color center ensembles at room temperature and 4K in HPHT, CVD and nanodiamond samples — •Kai Kühnlenz, Kevin Lauer, Phillip Kellner, Mario Bähr, Andreas T. Winzer, and Thomas Ortlepp — CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Deutschland

Nitrogen vacancy (NV) centers in diamond are key solid-state quantum emitters whose photophysical properties depend on their charge state and the surrounding diamond lattice. We analyze diamond samples made of chemical vapor deposition- (CVD), high-pressure-high-temperature- (HPHT) or nanodiamond material by exciting them with a 513nm green laser and detecting the fluorescence light via time resolved photoluminescence (TRPL). This work presents measurements of the fluorescence lifetime of NV-ensembles. Hereby a monochromator is employed to detect 20nm wide spectral bands centered at the NV- phonon sideband (710nm) and the zero-phonon-lines of NV- and NV0 (638nm and 575nm) to differentiate between the charge states. Measurements are performed at both room temperature (293K) and 4K. The influence of varying excitation laser power and of the selected spectral detection window is investigated and compared with established reference values. The measurement approach allows a systematic comparison of NV-diamond materials and provides a baseline for quantitative lifetime-based characterization of NV ensembles.

FM 7.2 Tue 9:45 BEY/0E40

Diamond windows for microwave application: numerical analyses and characterization by microscope and Raman measurements — •Gaetano Aiello, Andreas Meier, Theo Scherer, Sabine Schreck, and Dirk Strauss — Karlsruhe Institute of Technology, Institute for Applied Materials, 76021 Karlsruhe, Germany

Electron cyclotron heating and current drive systems in nuclear fusion devices feature optical quality polycrystalline diamond windows for the transmission of microwave beams of 1 to 2 MW power. The windows consist of diamond disks of 1 to 2 mm thickness integrated into a metallic housing. Numerical analyses verify the performance of such windows with respect to temperature and stress limits. In this work, examples of analyses are provided with reference to a Brewster-angle window design featuring a first-of-its-kind manufactured diamond disk with 180 mm diameter. For the first time, instead of a single constant value, the entire map of the loss tangent measured over the disk has been given as input to the analysis. In addition, examples of microscope and Raman investigations of the disks are shown with reference to dark microfeatures and residual stresses generated by the chemical vapour deposition process.

FM 7.3 Tue 10:00 BEY/0E40

Investigation of irradiation effects in artificial diamond — •Theo Andreas Scherer and Francesco Mazzocchi — Karlsruhe Institute of Technology KIT-IAM-AWP 76344 Eggenstein-Leopoldshafen

Diamond is used as window material for high power microwave transmission to heat plasmas and to perform diagnostics in nuclear fusion devices like ITER, Wendelstein 7X or ASDEX-UG. In such environments neutron and gamma radiation has a quite important influence on dielectric and thermal properties of diamond. Spectroscopic investigations, like RAMAN, cathode luminescence or EPR can detect all the defects produced by irradiation. Swift heavy ion and neutron irradiation was us to study defect chemistry and physics in diamond (single crystalline and polycrystalline diamond samples). Newest results of this investigation are presented.

FM 7.4 Tue 10:15 BEY/0E40

EC Heating systems for present and future fusion experiments and power plants — •Peter Späh — KIT, Institute for Applied Materials, Karlsruhe, Germany

CVD diamond windows are an essential component in Electron Cyclotron (EC) plasma heating and stabilisation systems for nuclear fusion reactors. Beside the characterisation and qualification of CVD diamond disks and the design and analysis of CVD diamond window assemblies, the Institute for Applied Materials (IAM) at Karlsruhe Institute of Technology (KIT) also contributes to concept findings, layout, design and integration of EC heating systems for several fusion experiments and power plant studies.

Experimental fusion devices and future fusion power plants with magnetic confinement require powerful heating systems for plasma core heating, plasma disruption mitigation, breakdown of gas, plasma ramp-up and -down, impurity control and to counteract thermal instabilities. Electron Cyclotron Resonance Heating (ECRH) is one of these heating systems. Microwave beams in the frequency range of 80 to 240 GHz are generated by gyrotrons and subsequently transmitted via waveguides and an antenna into the plasma chamber, where they interact with the electrons.

This talk gives an overview on the design status of the EC heating antennas for the EU DEMO fusion power plant and for the Volumetric Neutron Source (VNS) which is a conceptual study of a beam-driven Tokamak, serving as test-bed for full-sized breeding blanket modules.

coffee break

FM 7.5 Tue 10:45 BEY/0E40

Application of Raman and Photoluminescence Spectroscopy to MgO-C Refractories — •Julia Richter[1], Felix Drechsler[1], Till Stadtmüller[2], Cameliu Himcinschi[1], Christos Aneziris[2], and Jens Kortus[1] — [1]Technische Universität Bergakademie Freiberg - Institut für Theoretische Physik, Leipziger Straße 23, 09599 Freiberg, Germany — [2]Technische Universität Bergakademie Freiberg - Institut für Keramik, Feuerfest und Verbundwerkstoffe, Agricolastraße 17, 09599 Freiberg, Germany

By applying Raman and photoluminescence (PL) spectroscopy in the visible and near-infrared range to MgO, magnesia-carbon (MgO-C) refractory bricks - partially produced from recycled magnesia - are examined in hardened and coked state, and compared with nominally pure MgO powder as a reference. Two sharp, high-intensity PL signals (699 nm and 871 nm), each accompanied by symmetrical sidebands, are investigated by varying the excitation wavelength (532, 633, and 785 nm). The 699 nm PL feature observed for both brick and reference arises from Cr^{3+} impurities within the MgO lattices, whereas the 871 nm signal, associated with V^{2+}, appears only in the brick-derived MgO. To elucidate the origin of the symmetrical sidebands, temperature-dependent spectroscopic measurements from 100 to 295 K are performed, monitoring the intensity ratio of the higher-energy (anti-Stokes) and lower-energy (Stokes) sidebands. The results confirm phonon participation in both the MgO:Cr^{3+} and MgO:V^{2+} emission processes. Together, these findings connect fundamental defect physics with practical considerations in refractory material science.

FM 7.6 Tue 11:00 BEY/0E40

Creation of Color Centers in Magnesium Fluoride Single Crystals by Irradiation with MeV Heavy Ions — •Ayman El-Said — Physics Department and Interdisciplinary Research Center for Advanced Materials, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

The irradiation of ionic halide single crystals with MeV heavy ions can lead to the creation of various types of color centers [1]. Here, MgF2 single crystals were irradiated with MeV heavy ions of different energies and fluence [2]. UV-Vis spectroscopic measurements demonstrate the existence of F1-, F2-, and F3-centers due to ion irradiation. The type, concentration and creation efficiency of the observed color centers are studied in terms of ion fluence and energy loss. The results are not only of high importance for understanding the creation mechanism of the induced color centers but also for the degradation of optical materials in high-altitude and space environments.

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[1] K. Schwartz, C. Trautmann, A.S. El-Said, R. Neumann, M. Toulemonde, W. Knolle, Phys. Rev. B 70, 184104 (2004). [2] A.S.

El-Said, Rad. Phys. and Chem. 227, 112369 (2025).

FM 7.7 Tue 11:15 BEY/0E40

Oxygen vacancies in vanadium dioxide: A DFT+V study — •Oskar Leibnitz[1,2], Peter Mlkvik[1], Nicola A. Spaldin[1], and Claude Ederer[1] — [1]Materials Theory, Department of Materials, ETH Zurich, Switzerland — [2]Present address: Multifunctional Ferroic Materials, Department of Materials, ETH Zurich, Switzerland

We present a density-functional theory study of the effects of oxygen vacancies on the structural and electronic properties of vanadium dioxide (VO_2). Our motivation is the reported suppression of the metal-insulator transition by oxygen vacancies and the lack of a clear consensus on its origin. We use the DFT+V method with a static intersite vanadium-vanadium interaction term, V, to calculate the properties of the oxygen-deficient metallic rutile and insulating monoclinic M1 phases of VO_2 on the same footing. We find that oxygen vacancies induce local distortions in the M1 phase, but do not destroy the dimerization usually associated with the insulating behavior. In spite of this, we find that the M1 phase becomes metallic as a result of the partial filling of the conduction band due to a rigid-band-like doping effect.

FM 7.8 Tue 11:30 BEY/0E40

Distortion tensor around dislocations in GaN studied by electron backscatter diffraction and cathodoluminescence spectroscopy — •Domenik Spallek, Vladimir Kaganer, Oliver Brandt, Thomas Auzelle, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The effect of elastic distortion in the vicinity of a threading dislocation (TD) in GaN on its luminescence has been shown previously [1]. However, quantifying this distortion and its components remains a challenge. Therefore, we investigate individual TDs by correlated high-resolution electron backscatter diffraction (HR-EBSD) and cathodoluminescence (CL) spectroscopy. The sample is a high-purity, homoepitaxial GaN layer grown by molecular beam epitaxy with a low TD density.

A cross-correlation analysis with the software CrossCourt from BLG Vantage is used to determine the spatially-resolved components of the distortion tensor from the HR-EBSD results [2]. Signatures of the TDs are resolved in the elastic strain and rotation components. Through reference measurements, we explore the resolution limit of this analysis and its dependence on the material and measurement conditions. Hyperspectral CL maps show a reduced intensity as well as a shifted emission wavelength around the TD. With additional modeling of the distortion around a TD, these correlated measurements are related to the Burger's vector of the dislocation, determining its type.

[1] Kaganer *et al.*, Phys. Rev. Appl. **12**, 054038 (2019).
[2] Wilkinson *et al.*, Ultramicroscopy **106**, 307 (2006).