MM 11: Functional Materials: Performance, Reliability and Degradation

Time: Monday 17:00–18:15 Location: SCH A 215

MM 11.1 Mon 17:00 SCH A 215

Stability and electronic structure of NV centers at dislocation cores in diamond — •Reyhaneh Ghassemizadeh, Wolfgang Körner, Daniel F. Urban, and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

Due to its outstanding coherence properties, the negatively charged nitrogen-vacancy defect (NV center) in diamond is a promising system for quantum magnetometry and solid-state based quantum computing. However, its performance can be limited by the presence of crystal defects. We study the influence of dislocations on the stability and physical properties of the NV center within a density functional theory analysis [1]. We model the most common dislocations in diamond, namely the 30° and 90° partial glide, and calculate the defect formation energy, structural geometry, electronic defect levels and zero-field splitting (ZFS) parameters. Our simulations reveal that dislocations potentially trap NV defects with an energy release of up to 3 eV. In general, the properties of NV centers at dislocations show strong deviations with respect to their bulk values. However, the lowest energy configuration of a NV center at the core of a 30° dislocation shows very bulk-like properties. Its electronic level spectrum is only slightly modified and ZFS values deviate less than 5% from their bulk values. These results open the perspective to align multiple NV centers along this dislocation type with a linear-chain arrangement whose collective behavior may become advantageous for quantum technology applications. [1] R. Ghassemizadeh et al., Phys. Rev. B 106, 174111 (2022)

MM 11.2 Mon 17:15 SCH A 215

First-principles calculation of electroacoustic properties of wurtzite (Al,Sc)N — •Daniel F. Urban[1], Oliver Ambacher[2], and Christian Elsässer[1] — [1]Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany — [2]INATECH–Department of Sustainable Systems Engineering, University Freiburg, Germany

We study the electroacoustic properties of aluminum scandium nitride crystals $Al_{1-x}Sc_xN$ with the metastable wurtzite structure by means of first-principles calculations based on density functional theory [1]. We extract the material property data relevant for electroacoustic device design, namely the full tensors of elastic and piezoelectric constants. Atomistic models were constructed and analyzed for a variety of Sc concentrations $0 \leq x \leq 50\%$. The functional dependence of the material properties on the scandium concentration was extracted by fitting the data obtained from an averaging procedure for different disordered atomic configurations. We give an explanation of the observed elastic softening and the extraordinary increase in piezoelectric response as a function of Sc content in terms of an element specific analysis of bond lengths and bond angles.

[1] D. F. Urban, O. Ambacher, and C. Elsässer, Phys. Rev. B **103**, 115204 (2021)

MM 11.3 Mon 17:30 SCH A 215

Template-mediated well-defined nanostructure arrays for optical, electrical, and magnetic applications — •Rui Xu[1], Denys Makarov[1], and Yong Lei[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Ilmenau University of Technology, Ilmenau, Germany.

Advanced devices play a critical role for sustaining the ever-growing demands of our society for energy, information, health care, etc. To achieve high performance, devices with nanoscaled features are attracting more and more attentions by virtue of their unique and promising effects emerging at nanoscale. Structural design and engineering of materials provides a versatile platform to optimize the device performance and improve the commercial competitivity. Regarding the structural engineering, controlling the geometrical parameters (i.e., size, shape, hetero-architecture, and spatial arrangement) of nanostructures have been the central aspects of investigations and practical applications. By using anodic aluminum oxide template, we realized well-defined controlling of nanostructures over the size, in-plane/out-of-plane shape, hetero-architecture, and spatial arrangement. With such well-defined nanostructures, the optical, electrical, and magnetic performance of nanodevices can be obviously enhanced.

MM 11.4 Mon 17:45 SCH A 215

Advantages of oxygen-free wire-arc sprayed titanium coatings — •Maik Szafarska[1], Manuel Rodriguez Diaz[2], Cornelius Boekhoff[1], René Gustus[1], Kai Möhwald[2], Hans Jürgen Maier[2], and Wolfgang Maus-Friedrichs[1] — [1]TU Clausthal, Clausthal Centre of Material Technology — [2]Leibniz Universität Hannover, Institut für Werkstoffkunde

Typically, thermal spraying is carried out in air, with compressed air acting as the cooling agent. However, the application of oxygen-affinitive materials like titanium is heavily influenced by the oxygen content in the atmosphere. Besides the impact on chemical composition, it can negatively influence the wetting behavior of the surface, the residual stress inside the coating and the formation of cracks and defects. Alternatives like cold gas spraying and vacuum plasma spraying grant only slight improvements coupled with an increased difficulty or cost for industrial use. Using silane-doped argon, it is possible to reduce the oxygen partial pressure to extremely low levels well below 10E-23 mbar. This makes application of wire-arc spraying possible for oxygen-affinitive materials like titanium. The titanium coatings feature a significantly reduced porosity caused by improved wetting behavior of titanium particles during the spraying process. Additionally, the coatings show extremely high adhesive tensile strengths compared to coatings formed in air. Discussed topics include particle formation, surface morphology and chemical composition, splat profiles, coating cross sections and interfacial diffusion between titanium coatings with iron-substrates.

MM 11.5 Mon 18:00 SCH A 215

Simulative study on crocheted fabrics via finite element method — •Jan Lukas Storck[1], Dennis Gerber[1], Liska Steenbock[1], and Yordan Kyosev[2] — [1]Bielefeld University of Applied Sciences, Bielefeld, Germany — [2]Technische Universität Dresden, Dresden, Germany

Crochet is a rarely studied but very versatile textile technology. Industrial production of crochet does not yet exist but approaches to automation have recently emerged. In order to research the properties of crocheted fabrics by simulation, the finite element method (FEM) is well suited as a numerical approach due to the high complexity of the crochet structure. To the best of our knowledge, the FEM study presented here is the first one on the basic mechanical properties of crocheted fabrics [1]. A topology based key point model of an exemplary crocheted fabric at the meso scale was developed and studied with LS-DYNA (Livermore Software Technology Corporation). Displacements in the two textile directions (course and wale) revealed an even distribution of stresses in the fabric, whereby the stresses in course direction propagated faster. This and the differing stitch deformations show anisotropic properties. Such fast-calculating FEM simulations in combination with the developed flexible modelling can also be used in the future for engineering crocheted textiles for technical applications.

Reference [1]: J. L. Storck, D. Gerber, L. Steenbock, Y. Kyosev. Topology based modelling of crochet structures. Journal of Industrial Textiles, 2022, accepted, doi: 10.1177/15280837221139250.