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Neutron diffraction from Boro-carbon for efficient structural analysis and defect detection

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Neutron scattering is considered to be a complimentary technique to electron microscopy which unveils detailed information on the defect structure in real space over tiny localised volumes in the specimen. Boron-doped diamond (BDD) is a conductive material and is considered as a potential candidate for electrode materials with large cell voltages. However the exact role of Boron and its location within the crystal has not been investigated so far. Within the scope of this PaNOSC user case, inelastic neutron scattering experiments and ab-initio calculations have been used to investigate the location-dependent response of defects in diamond, and BDD structures. Ab-initio tools from atomistic simulation environment (ASE) is used for obtaining structural and electronic properties, and relaxed nuclear positions. Based on these nuclear positions, neutron scattering is simulated with McStas code in well-known experimental environment.

The origin of the diffraction peaks was identified, correlating them to individual system geometries. Our approach can correlate the appropriate 'micro atomistic scenario'among a manifold of possibilities to reproduce the observed 'experimental macro features'.

Presenter: UPADHYAY KAHALY, Mousumi (ELI-ALPS)