Jožef Stefan Institute
Ljubljana, Slovenia | K7 / Department for Nanostructured Materials

VIRTUAL SEMINAR

Thursday, 21.04.2022 at 13:00

Structural analysis of basal-plane inversion boundaries in Sn4+ and Sb5+ doped zinc oxide

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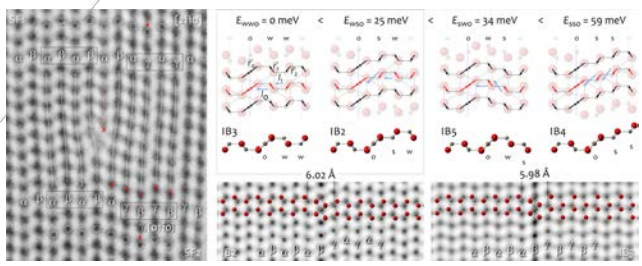
Chemically–induced planar defect structures and domain boundaries are of a great importance in the design of diverse functional materials, since they can be used to tailor phonon scattering, electrical conductivity, optoelectric, piezo or magnetic properties. While most of the impact is reflected through engineering of the electronic structure, they are also known to be effective in controlling crystal growth and morphology. Basal–plane head–to–head inversion boundaries (IBs) in SnO_2– and Sb_2O_3–doped ZnO were examined due to their discontinuous effects in phonon scattering, electron transport, and even p–type conductivity of ZnO. It is known that the incorporation of specific dopants with the oxidation state higher than 2+ triggers polarity inversion in the wurtzite ZnO through the formation of IBs. Even though IBs are known since the early 1990s, there are still unresolved issues and open questions related to their structure. Here, I combined advanced experimental and theoretical methods to solve the structures of IBs in Sb_2O_3 and SnO_2–doped ZnO, with a special focus on their translation states and in–plane cation distributions. Sb–rich IBs were used to characterize the decisive structural elements defining the IB translation states, while in Sn–rich IBs the in–plane cation ordering was investigated. Different IB models were designed and were further examined by DFT (Density functional theory) calculations to determine their stability and energetic contributions. This was followed by a systematic reexamination of IBs in SnO_2– and Sb_2O_3–doped ZnO ceramic samples using quantitative HRTEM (High-resolution transmission electron microscopy) and STEM (Scanning transmission electron microscopy) methods and quantified via model–based image simulations and correlation.

The implemented methodology combining atomic–scale microscopy with structural modeling and *ab initio* calculations has the capacity to predict fine structural details with confidence levels down to <1 pm.



Kindly invited.