Disconnections : from cubic to orthorhombic crystals in ionic systems

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Résumé pour : poster

Disconnections are line defects in grain boundaries (GB) combining dislocation and step characters. While they have initially been used to explain the GB shear coupling phenomenon, the nucleation and the motion of these defects have been extensively studied in the last years for their critical role on GB dynamic properties. Nevertheless, the majority of the studies on disconnections focused on simple materials such as faced centered cubic metals.

In this poster, we will present a molecular static study of the energetic of disconnection dipoles in two ionic crystals, MgO periclase having a cubic structure and Mg_2SiO_4 forsterite having an orthorhombic symmetry. By computing the energy of the dipole as a function of disconnection distance we will show that the dipole energy is strongly dependent on the state of the GB (called complexion). We will also show that dipole energy is extremely high in forsterite which may explain why GB shear coupling had never been observed neither experimentally nor numerically in this material.