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2021.03.05 (Fri.) 16:30 ~

Venue: Zoom
A link will be sent @grc-all within 30 minutes before the beginning of the seminar.

First-principles investigation of tilt grain boundaries in (ferro)periclase

Ferropericlase is the second most abundant phase of Earth's lower mantle and is also considered to be one of the main constituents of super-Earth's mantles. Ferropericlase is more ductile compared to mantle silicates and is likely to affect the bulk rheology of mantle aggregates, controlling the dynamics of planetary interiors such as the Earth. The properties of grain boundaries are critical to describe the mechanical behavior of polycrystalline aggregates. Despite previous work on MgO grain boundaries, little is yet known about the properties and mobility of ferropericlase grain boundaries at pressure conditions of deep planetary interiors.

In this study, I carried out atomistic simulations based on the density functional theory to model the structures, energies and iron spin states of a series of [001] symmetrical tilt grain boundaries in periclase as a function of pressure. By determining the segregation energies of iron, it is shown that iron prefers specific grain boundary sites which changes the local spin transition of iron with respect to bulk ferropericlase. I then investigated the mechanical behavior of the Σ5 tilt grain boundary by applying simple shear increments to the simulation cell in order to increase the stress on the interface, needed to trigger the migration of the grain boundary. Here, I will present the mechanisms of grain boundary migration and the evolution of the ideal shear strengths up to a pressure of 400 GPa. Implications for the deformation of (ferro)periclase at conditions of Earth's and super-Earth's mantles will be finally discussed.

Keywords:
1. Grain boundaries
2. (Ferro)periclase
3. Mechanical behavior