

Electrical conductivity of serpentine fluids at subduction zone conditions

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Owing to pervasive faults, sea water interacts with oceanic crusts and stabilizes a suite of layered hydrous silicate phases. As the oceanic crusts subduct, the hydrous phases are also dragged along with the subducting slab. These hydrous phases have limited thermal stabilities and they eventually dehydrate, releasing fluids. These fluids are less buoyant and hence migrate upwards. The fluids interact with the overlying mantle wedge. These released fluids rehydrate the mantle wedge i.e., rehydrates peridotitic mantle and stabilizes serpentine. From geophysical observations, the mantle wedges of subduction zone are characterized by low seismic velocities and electrical resistivities. In order to assess the role of fluids and serpentine, we have measured the electrical conductivity of natural serpentinites at pressure (2 GPa) and temperatures (up to 1000 K) relevant to mantle wedge conditions. Among the two natural serpentine sample investigated, one contained antigorite and traces of carbonate and the other contained chrysotile and carbonate. We distinguish the various polytypes of serpentine by careful analysis of the crystal structure using transmission electron microscopy (TEM). The measured conductivity of serpentine (10^{-4} Sm^{-1}) is higher than anhydrous olivine (10^{-6} Sm^{-1}) by two orders of magnitude at 1000 K. Upon dehydration, serpentine releases fluids which were also measured in our experiment and showed a very high conductivity of the order of 10^{-2} - 10^0 Sm^{-1} range. This can easily explain the high conductivities observed in many subduction zones.

Epitaxial garnet-muscovite interfaces: Molecular modelling

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Introduction

Computer simulations of garnet-muscovite interfaces provide a means of assessing the importance of interfacial energetics to epitaxial nucleation. Experiments and natural samples provide information about specific grain boundary orientations and their prevalence and invite speculation on the importance of particular orientations, but the determination of grain boundary energies from these data is difficult. Currently, there are few constraints on the interfacial energies of naturally occurring minerals and no studies have focused on garnet, a mineral that is of great significance to the metamorphic community. Combining data on grain boundary orientations from natural and experimental samples with molecular modelling that uses energy minimization allows for the determination of relative energies for naturally-occurring grain boundaries between garnet and muscovite.

Methods

Force-field simulations are particularly well-suited to the task of calculating grain-boundary energies for a specific set of conditions; here the General Utility Lattice Program (GULP) simulation code is employed for this purpose [1]. A 2-D periodic slab model is used to investigate muscovite-garnet interfaces. Here each phase is represented by two regions: an interfacial region in which the atoms are fully relaxed, in contact with a second rigid region that represents the underlying bulk material. The two unconstrained regions of garnet and muscovite are then placed in contact to create the interface, while the bulk regions are allowed to rigidly translate relative to each other in order to minimize the total energy. The total potential energy of this final configuration is compared to that of the two bulk structures and by dividing the difference between the two by the area of the interface, an interfacial energy is calculated. The parameters used to describe the energetics of the muscovite and garnet structures include Buckingham potentials, an oxygen core-shell spring constant, a three-body term to describe the O-Si-O bonding angle, and a Morse bond to describe the H-O bond [2,3].

Results

Initial simulations indicate that a garnet slab six unit cells thick and a muscovite slab five unit cells thick are sufficient for simulating the $(110)_{\text{grt}} \parallel (001)_{\text{ms}}$ with $[100]_{\text{grt}} \parallel [100]_{\text{ms}}$ interface. Additional simulations reveal that certain surface terminations of the muscovite and garnet slabs create more stable surfaces to be used in the garnet-muscovite interface simulations. The stability of these surfaces may be a guide to determining the precise interfaces between garnet and muscovite in natural samples.

[1] Gale & Rohl (2003) *Molecular Simulation* **29**, 291-341. [2] Steele *et al.* (2000) *Geochimica et Cosmochimica Acta* **64**, 257-262. [3] van Westrenen *et al.* (2000) *Geochimica et Cosmochimica Acta* **64**, 1629-1639.