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Mechanism of Olivine-Spinel Transformation and Microstructural Development under Differential Stress by Phase Field Method

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Olivine is the most abundant material in the upper mantle and undergoes phase transformation to wadsleyite and ringwoodite at about 410 km and 520 km depths, respectively. The phase transformation affects the mantle rheology (e.g. deep-focus earthquake and slab deformation). There are two nucleations during the olivine-spinel transformation (intra-crystalline nucleation and nucleation at the grain boundary). However, the physicochemical process of olivine-spinel phase transformation is not clear. Previous studies suggested the mechanism of the nucleation vary depending on the difference of magnitude of differential stress and the deviation of pressure- and temperature-conditions from the phase boundary. Although we need to conduct deformation experiments at relevant conditions for the olivine-spinel phase boundary in the subduction plate, it is difficult to conduct such experiments under high pressure. Many researchers have conducted the experiments using germanate olivine as an analogue material. Thus, it is useful to conduct numerical experiments which are capable of treating large grain size and slower strain rate close to the natural condition. We adopt Phase Field Model (PFM) to model microstructural development associated with olivine-spinel phase transformation under differential stress condition. In the PFM, we configure the order parameter which describes the distribution of two phases. The phase boundary is described as a field where the order parameter continuously changes between two phases. Therefore, PFM is a powerful tool for the simulation of microstructural development with complex morphological features. Using, the PFM, we conduct numerical experiments at conditions of confining pressures of 1 $\sim$ 5 GPa, temperatures of 1000 K $\sim$ 1400 K, strain rate of $10^{-4}\sim$ 10^{-7} s^{-1}, with a various grain size ranging from 100 μm to 1 mm under various ranges of differential stresses. We reveal that under differential stress less than 1 GPa, intra-crystalline nucleation is dominant when P-T conditions are close to the (germanate) olivine-spinel phase boundary, while nucleation at the grain boundary is dominant when P-T conditions are far away from the phase boundary. However, under high differential stress like 2 $\sim$ 3 GPa, the volume fraction of spinel by nucleation at the grain boundary is much larger than that by intra-crystalline nucleation. Therefore, we can point out that, under high differential stress condition, nucleation at the grain boundary may be dominant regardless of the distance from the phase boundary. The volume fraction of spinel by both nucleations at the initial grain size of 1 mm is much less than that at the initial size of 100 μm. Meanwhile, the volume fraction at strain rate of 10^{-6} s^{-1} and 10^{-7} s^{-1} is more than that at strain rate of 10^{-4} s^{-1}. These indicate that the effect of differential stress is large for and the magnitude of differential stress is a critical parameter which decides the mechanism of olivine-spinel phase transformation. Also, the volume fraction of spinel is sensitive to the initial grain size. Therefore, while slabs are subducting, the magnitude of differential stress and initial grain size decide the mechanism of olivine-spinel phase transformation.