Constraints on interfacial energy from Phase-field modeling of grain growth in olivine aggregates

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Segregation and migration of melts in magmatic systems depend critically on dihedral wetting angles and, therefore, on Interfacial energies of mineral surfaces. Grain boundary energies of different surfaces of olivine control the extraction of melts from mantle lithologies. In spite of this there exists only one direct experimental measurement (Cooper, R.F. and Kohlstedt, D.L. Adv. Earth Planet. Sci. 12, 217-228, 1982) of this quantity due to experimental challenges. But the impact of differences in interfacial energy between different surfaces on overall melt permeability has been documented (Huang et al., American Mineralogist, 108: 2244 - 2259, 2023). We have combined grain growth experiments with Phase Field modelling to extract the relative interfacial energies during grain growth. We have carried out grain growth experiments on olivine aggregates (Mg₂SiO₄ + 2vol.%MgSiO₃ between 1150-1390°C from 30min - 76hrs in air) to separate the effect of temperature and time on grain growth and the grain boundary plane distribution (GBPD, a proxy for the relative grain boundary energies). We combined these observations with a Phase field model developed to describe the anisotropy of surface energies. The relative variation of olivine surface energies was defined to describe the known olivine habit accurately. The evolution of a system with initial olivine nuclei placed randomly in space and orientation and allowed to evolve by free energy minimization was used to explore the impact of anisotropic surface energies on grain growth behavior. Our threedimensional phase-field modelling results were compared directly with experimental datasets, including the evolution of grain size, grain size distributions, misorientation distributions, and grain boundary plane distributions (GBPD) for olivine polycrystals annealed under different thermal and temporal conditions. These provide preliminary constraints on relative surface energies of olivine relative to (001), taken to be unity: (100) = 0.5, (010) = 1.67, (101) = 0.83, (110) = 2.33 and (121) = 0.832.26 times the surface energy of (001). Further refinement and incorporation of such anisotropy in melt migration models would considerably improve our understanding of anisotropy of melt location and flow as well as the development of textural features of olivine-bearing rocks, which may be related to seismic signals.

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