EGU2020-21694, updated on 02 Dec 2022
https://doi.org/10.5194/egusphere-egu2020-21694
EGU General Assembly 2020

The role of grain boundary energy anisotropy on the grain size evolution during normal grain growth.

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Many regions of the Earth's mantle deform in grain size-sensitive creep regimes. The grain size right below the transition zone is believed to be very small, and the grain size should in subsequent depths be mainly controlled by normal grain growth. The grain size evolution is commonly predicted using either existing grain growth laws in combination with grain boundary diffusion coefficients or by extrapolating empirically determined grain growth laws. Effects of Zenner pinning and different ratios of second phases have been studied, while the role of anisotropic grain boundary properties is currently neglected[1]. The grain boundary energy varies with the orientation of the grain boundary plane, as expressed through the typical crystal habitae (Wulff-shapes). Individual crystals in a polycrystalline material maintain a grain boundary energy anisotropy during grain growth. Here we study how grain boundary anisotropy impacts grain boundary migration and normal grain growth rates by three-dimensional phase-field simulations[2]. We imply grain boundary energy minimization by faceting/varying the grain boundary plane to minimize the grain boundary energy. The ideal grain boundary energy anisotropy for the solid-solid interface is taken from experimentally investigated grain boundary plane distributions and grain boundary energy distributions on periclase (MgO). We compare the grain size evolution in simulations with isotropic and anisotropic grain boundary energy of cubic crystal symmetry. We found that the grain boundary energy anisotropy has a significant influence on grain boundary migration and grain growth kinetics[2].

$\langle r\rangle^2 - \langle r_0\rangle^2 = kt$

The change in grain size is given as variation between the initial and final average grain radius, r. The time is t, and a material-specific parameter that accounts for the grain boundary energy anisotropy is extracted from the simulations as

$k = A \cdot \mu_{gb} \cdot \sigma_{gb}$

Where, the grain boundary energy, σ_{gb} varies with orientation, and the grain boundary mobility, μ_{gb} *assumed to be isotropic.* We found that the rate of grain growth for periclase, A is a factor of 3 smaller compared to an isotropic material.

These results are of three-fold importance:

A better prediction of grain size evolution will need to develop an anisotropic theory for grain growth, that address our lake in knowledge regarding pressure effects on both grain boundary energy anisotropy and diffusion.

1. Rohrer, G. S. Annu. Rev. Mater. Res. 2005

2. Salama et al. Acta Materialia 2020