Full field modeling of grain growth in mantle rocks based on a level-set enhanced finite element framework

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In naturally deformed mantle rocks, a switch from grain size insensitive (GSI) to grain size sensitive (GSS) creep by decreasing grain size can explain the initiating or enhancing of strain localization at zones of low grain size. The long-lived nature of these weak zones in Earth conditions despite the relatively high lithospheric temperatures leads us to investigate the kinetic of peridotites grain growth.

We choose to initiate this study of microstructure evolution within a numerical simulation context closely coupled with the various pre-existing experimental results for mantle rocks. Several full field modeling techniques have been developed in order to compute rock microstructural evolutions, however, the numerical approach that we propose has not been used in the context of geomechanics. This numerical approach is based on an implicit description of the interfaces by using level-set functions within a finite element framework. This approach has successfully been applied to study complex microstructural evolutions phenomena present in metals.

This numerical context allows to account for different mechanisms (e.g. grain boundary migration, Zener-pinning) within the same formalism, making it a robust, adaptable and scalable code. Moreover, recent numerical developments had considerably increase the numerical efficiency of the code permitting 3D modeling for much lower computational costs.

The physical parameters needed to investigate grain growth (mobility and energy of a grain boundary) had been obtained from experimental data and are available in literature. Our full field simulations have been compared with those experimental results, showing a good agreement in terms of microstructure and grain growth kinetic. Furthermore the numerical approach proposed allows to account for more complex mechanisms such as secondary phase particles pinning or even recrystallization (among many others).

The potential of this full field technique is tremendous, since it allows to numerically calibrate mean field models (such as generalized Burke and Turnbull or modified versions of the classical Zener equation). This might allow to run0 large scale simulations taking into account variations of grain size accurately computed by mean field models correctly calibrated within the lithospheric conditions.

Keywords: Grain growth modeling, Full field models, Finite elements, Mean field models