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Numerical simulations of grain boundary migration and melt topology and transport in a stressed partial melt

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Grain boundary migration is one of the most important processes that can change a microstructure under static conditions. The movement of grain boundaries depends on the grain boundary surface energy and mobility. If a liquid phase, like a melt, is also present in the aggregate, an order of complexity is added, since above a certain percentage, the melt is interconnected by tubes or channels that allow rapid transport within or out of the aggregate. Under static conditions, i.e. crystallization and annealing, the melt has a defined wetting angle at triple junctions (where two solid grains are in contact with melt).

Contrary to what is commonly assumed, our numerical simulations show that the wetting angle is not a constant but is dynamically adjusted during the evolution of a microstructure. This was also observed in analogue experiments by Walte and Bons (unpublished). This has implications for the rate at which a microstructure can adjust to other influences such as stress, since the boundary movement can be significantly slower (or faster) in the presence of melt. Furthermore, melt pockets can be over- or under-pressured. Under-pressured melt pockets will try to gain melt from surrounding melt pockets if they are interconnected and/or will react by decreasing their area. Over-pressured melt pockets can either increase their area or loose melt to other, connected under-pressured melt pockets. While this happens, the wetting angles can be significantly different from the equilibrium angle, which itself strongly influences the connectivity. However, if the overpressure reaches a certain threshold, the microstructure will fail by fracturing, suddenly changing the melt transport properties of the aggregate.

The complex interaction and coupling between stress, melt pressure, wetting angle, connectivity and permeability determine the segregation and accumulation of melt from a partially molten source rock. With our numerical simulations we show that all these factors have to be taken into account and that the process cannot be described using simple models with a static wetting angle.