

Ti resetting in quartz during dynamic recrystallization: Mechanisms and significance

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ABSTRACT

The ubiquity of quartz in continental crust, and the involvement of SiO₂ in multiple metamorphic processes such as reactions, fluid flux, and solution-transfer processes, makes quartz an obvious choice for reconstructing prograde metamorphic conditions in various rock types. Recent studies have shown the usefulness of analyzing Ti distribution in quartz to constrain pressure-temperature-(relative) time-deformation (*P-T-t-D*) in metamorphosed tectonites. New high-precision single-crystal X-ray diffraction volume constraints on Ti-doped and chemically pure quartz provide further evidence for substitution of Ti⁴⁺ for Si⁴⁺ in the tetrahedral site in quartz, with resultant lattice strain on the structure.

Recent applications of the Ti-in-quartz thermobarometer to dynamically recrystallized quartz have identified recrystallized subgrains that contain lower Ti concentrations ([Ti]) than their host porphyroclasts. In addition, [Ti] are lower than expected for the temperatures of recrystallization. Atomistic simulations that estimate energetic perturbations resulting from Ti incorporation into the quartz lattice indicate that significant increases in strain energy occur only at very high [Ti]; the strain-energy increase is negligible for [Ti] typical of quartz grown under mid-crustal conditions. This suggests that lattice strain rarely provides an appreciable driving force for Ti loss from quartz; instead, it appears that subgrain boundaries and dislocation arrays migrating through recrystallizing quartz crystals can promote localized re-equilibration, thermodynamically regulated by the composition of the intergranular medium (typically undersaturated in Ti). It therefore appears that analyses from dynamically recrystallized quartz cannot be meaningfully interpreted until methods are developed that can account quantitatively for the reduction of Ti resulting from crystal plastic flow.

Keywords: Titanium, quartz, dynamic recrystallization, lattice strain, atomistic simulation