# A microscopic view of nucleation in the anatase-to-rutile transformation

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We use molecular simulation techniques to investigate the anatase-to-rutile transformation in Titania nanocrystals. A thermodynamic analysis indicates that edge and corner atoms significantly influence the critical size at which rutile nanocrystals become energetically preferred over anatase. Using molecular dynamics simulations, we probe kinetics of the transformation in individual anatase nanocrystals and in nanocrystal aggregates. We follow structural evolution using simulated X-ray diffraction. Additionally, we develop a local order parameter to distinguish individual Ti ions as anatase, rutile, or anatase {112} twin-like. We apply our local order parameter to track the formation and growth of rutile nuclei. Anatase {112} twins form easily at surfaces and interfaces of nanocrystal aggregates and rutile nucleates among the twins. Stable rutile nuclei maintain {101} facets during growth, as a result of nucleation from layers of alternating anatase {112} twins. Our results are in agreement with experiment and indicate the central role of {112} twin-like anatase in the transformation.
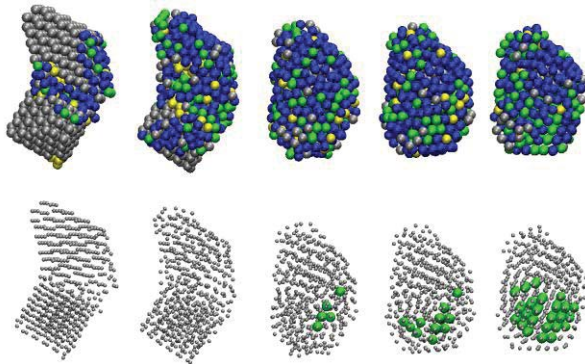

Figure 1: Structural evolution of an aggregate during transformation at 1473 K. Upper row: only Ti ions in the aggregate are shown, with anatase ions in silver, anatase {112} twins in blue, rutile in green, and undefined ions in yellow. Lower row: Ti ions in the stable rutile nuclei are in green and magnified, all other Ti ions are shown in silver.

Temporal changes in magma geochemistry in the northern Lhasa Terrane, Tibet: Response to the Lhasa–Qiangtang collision

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Magma generation and evolution is a natural consequence of mantle dynamics and crust-mantle interaction. As a result, magma compositional variation in time and space can be used, in turn, to infer these deep processes. Indeed, the Baingoin Batholith, the largest batholith in the northern Lhasa Terrane, manifests this efficacy. This batholith was emplaced in response to the Lhasa–Qiangtang continental collision (ca. 140–110 Ma). Our data indicate that it was emplaced in three distinct pulses (i.e., 132 ± 2, 121 ± 3, and 113 ± 3 Ma) rather than in a single phase (ca. 121 Ma), as previously thought, and that its magma chemistry changed through time (Figure 1). The 132 ± 2 Ma samples are silica-rich and have small whole-rock ε_{Nd} (t) (−2.7 to −2.4), positive zircon ε_{Hf}(t) (+2.3 to +11.0), low zircon $\delta^{18}O$ (5.81–7.16 ‰) values, and low Ti-in-zircon temperatures (T_{Ti}^{zir} = 630–660°C). The 121 ± 3 Ma samples are compositionally diverse and show varying ε_{Nd}(t) (−10.0 to −4.8), decreased zircon ε_{Hf}(t) [−8.5 to +5.9], increased zircon $\delta^{18}O$ (7.42–9.52 ‰), and increased T_{Ti}^{zir} (ca. 650–750°C) relative to the 132 ± 2 Ma rocks. The 113 ± 3 Ma samples have similar ε_{Nd}(t) (−9.5 to −4.8) and T_{Ti}^{zir} (ca. 680–750°C) but slightly increased zircon ε_{Hf}(t) (−7.1 to +6.4) with varying zircon $\delta^{18}O$ (6.25–11.12 ‰) relative to the 121 ± 3 Ma rocks. Similar changes of magma geochemistry are also present in the coeval magmatic rocks from Yanhu (Figure 1). It is evident that the parental magmas of the 132 ± 2 Ma rocks originated from hydrous partial melting of juvenile crust. Progressive incorporation of ancient crustal material into the source region of the 121 ± 3 Ma rocks coincided with the involvement of the subducting Qiangtang continental crust or the contamination of the Lhasa basement-derived melts during the Lhasa–Qiangtang collision. The significant input of mantle-derived component in the 113 ± 3 Ma rocks may have resulted from slab breakoff-induced magmatism and related mantle melting events, following the final Qiangtang–Lhasa amalgamation.
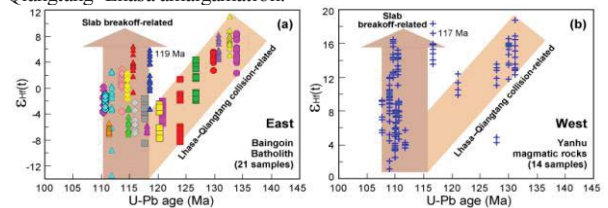
Figure 1: Space-time variations of zircon ε_{Hf}(t) of Early Cretaceous magmatic rocks from the northern Lhasa Terrane, central Tibet