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Atomic structure and formation mechanism of (101) rutile twins from Diamantina (Brazil)

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Abstract

We studied the atomic structure and the chemical composition of (101)-type rutile (TiO_2) twins from Diamantina in Brazil by electron microscopy methods to resolve the mechanism of their formation. The twin boundaries were studied in two perpendicular orientations to reveal their 3D structure. The presence of a precursor phase, such as Al-rich hydroxylian pseudorutile (HPR; kleberite), during the initial stages of the crystallization appears to be the necessary condition for the formation of (101) twins of rutile at this locality. The precursor with a tivanite-type structure serves as a substrate for the topotaxial crystallization of rutile. Depending on the initial crystallization pattern the rutile can grow either as a single crystal or as a twin. During the progressive crystallization of the rutile Al-rich oxyhydroxide (diaspore, α-AlOOH) clusters are concentrated at the center of the precursor where they are pinned to the twin boundary as the precursor is fully recrystallized into rutile. At the increased temperatures the remaining diaspore precipitates are converted to corundum (α-Al_2O_3), while the two crystal domains continue to grow in the (101) twin orientation. In addition to the primary (101) twin, series of secondary {101} twins are formed to accommodate the residual tensile stress caused by the diaspore-to-corundum transformation. Based on the observed corundum-rutile $[0001]_C(11\bar{2}0)_C||[010]_R(101)_R$ and ilmenite-rutile $[0001]_I(1\bar{1}00)_I||[010]_R(301)_R$ crystallographic relations a unified mechanism of the genesis of the {101} and {301} reticulated sagenite twin clusters is proposed.

Keywords: Rutile, alumina, dehydration, exsolution, mobility, epitaxy, twinning