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Atomic structure and formation mechanism of (301) rutile twins from Diamantina (Brazil)

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Abstract

Rutile (TiO_2) twins from Diamantina in Brazil were investigated using analytical transmission electron microscopy methods. High-resolution transmission electron microscopy (HRTEM) imaging of (301) twinned rutile revealed the existence of a coherent interlayer at the twin boundary. The interface lamella, with a lateral width of a few nanometers, consists of ilmenite ($FeTiO_3$) containing some Al. The orientation relationship between the ilmenite lamella and the epitaxial rutile crystals is $(01\bar{1}0)[0001]_I \parallel (301)[010]_R$. The ilmenite-rutile interfaces are atomically sharp and devoid of misfit dislocations that would compensate for the lattice mismatch between the two structures. The Ti/Fe concentration ratios, as measured in the twin lamella by means of the variable-beam-diameter energy-dispersive spectroscopy (VBD/EDS) technique, correspond to ilmenite. The valence-sensitive features in electron energy-loss spectra (EELS) revealed that the Fe in the twin lamella adopts a divalent oxidation state (Fe^{2+}), which is characteristic of ilmenite. The lattice mismatch between the ilmenite and rutile appears to be compensated by the incorporation of Al into the ilmenite. The presence of goethite-related reflections and the existence of nanotwins in the ilmenite lamella imply that it formed via a thermally induced dehydration process from an oxyhydroxide precursor mineral with a tivanite-type structure. This lamella subsequently served as a nucleation site for the epitaxial growth of rutile domains in a (301) twin configuration.

Keywords: Rutile, ilmenite, corundum, hematite, epitaxy, twinning