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Structural investigation of (130) twins and rutile precipitates in chrysoberyl crystals from Rio das Pratinhas in Bahia (Brazil)

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Abstract

We studied V-shaped twins of chrysoberyl ($BeAl_2O_4$) from Rio das Pratinhas pegmatites near Arataca in the Bahia state of Brazil. The local structure of the twin boundaries was determined using powder X-ray diffraction analysis (XRD), transmission electron microscopy (TEM) methods, and density functional theory (DFT) calculations. To provide the most reliable model for DFT and HRTEM simulations the structure of chrysoberyl was first refined in the orthorhombic space group 62 (*Pmnb*) with unit-cell parameters: a = 5.4825(1) Å, b = 9.4163(2) Å, and c = 4.4308(1) Å, with 0.5 at% of Fe^{3+} present on the Al(2) sites, suggesting an average composition of $BeAl_{1.99}Fe_{0.01}O_4$. TEM study of V-shaped twins showed that the twin boundary lies in the (130) planes, and the angle measured between the crystal domains related by mirror twin operation is ~59.5°. Rigid structural model of (130) twin boundary in chrysoberyl was refined by DFT calculations, using a pseudo-potential method. The twin boundaries show local enrichment with Ti. Bulk chrysoberyl contains numerous nanosized TiO_2 precipitates with a distorted rutile structure, following the orientation relationship of $[001]_{Ch}\{120\}_{Ch}||[010]_R\{103\}_R$. The increase of Ti at the twin boundaries and the formation of rutile-type TiO_2 precipitates in bulk chrysoberyl suggest a transient Ti-exsolution that took place after the twin formation.

Keywords: Chrysoberyl, alexandrite, Rietveld analysis, atomic structure, twinning, topotaxy