Crystal structure of new polymorph of Sr_2TiO_4 with tetrahedral titanium

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Sr_2TiO_4, first member of the Ruddlesden-Popper series $Sr_{n+1}Ti_nO_{n+1}$, has been long known to undergo a phase transition at 1550 °C. This transition makes the growth of single crystals of this material highly challenging, because it usually breaks the crystal into a periodic array of uneven lamellae. While the low temperature tetragonal phase is widely studied due to its close connection to the famous perovskite $SrTiO_3$, there is little information about the high temperature α—phase.

We stabilized the high-temperature $\alpha-Sr_2TiO_4$ crystals by rapid cooling of the melt from temperature above the structural transition. The α—phase crystallizes in the orthorhombic $Pna2_1$ group and is isostructural to the orthorhombic forms of Sr_2VO_4 and Sr_2CrO_4. Its structure is formed by a complicated framework of large SrO_x polyhedra with tetrahedral cavities occupied by the transition metal. The tetrahedral coordination of Ti^{IV} makes the $\alpha - Sr_2TiO_4$ quite a rare case among titanate compounds, the only other known example being the barium orthotitanate Ba_2TiO_4 [1].

In this work, we report the crystal structure of the high-temperature phase of Sr_2TiO_4. We compare the optical properties of related compounds and discuss possible mechanism driving the structural transition.

[1] Gunter, J., Jameson, G. (1984). Acta Cryst. C40, 207.