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Crystal chemistry and thermodynamic properties of zircon structure-type materials

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Abstract

Zircon-class ternary oxide compounds have an ideal chemical formula of ATO_4, where A is commonly a lanthanide and an actinide, with T = As, P, Si, or V. Their structure ($I4_1/amd$) accommodates a diverse chemistry on both A- and T-sites, giving rise to more than 17 mineral end-members of five different mineral groups, and in excess of 45 synthetic end-members. Because of their diverse chemical and physical properties, the zircon structure-type materials are of interest to a wide variety of fields and may be used as ceramic nuclear waste forms and as aeronautical environmental barrier coatings, to name a couple. To support advancement of their applications, many studies have been dedicated to the understanding of their structural and thermodynamic properties. The emphasis in this review will be on recent advances in the structural and thermodynamic studies of zircon structure-type ceramics, including pure end-members [e.g., zircon ($ZrSiO_4$), xenotime (YPO_4)] and solid solutions [e.g., $Er_xTh_{1-x}(PO_4)_x(SiO_4)_{1-x}$]. Specifically, we provide an overview on the crystal structure, its variations and transformations in response to non-ambient stimuli (temperature, pressure, and radiation), and its correlation to thermophysical and thermochemical properties.

Keywords: Zircon, thermodynamics, crystal chemistry, high pressure, high temperature, lanthanides, actinides