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Review of Crystal Chemistry and Thermodynamic Properties of Zircon Structure-Type Materials

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Zircon-type minerals are common as accessory phases, which occur in a variety of sedimentary, igneous, and metamorphic rocks. Zircon structure-types are ternary oxides with an ideal chemical formula of ATO_4 ($I4_1/amd$), where usually A are lanthanides and actinides, with T = As, P, Si, V. This structure accommodates diverse chemistry on both A- and T-sites, giving rise to more than seventeen mineral end-members of five different mineral groups, and forty-five synthetic end-members. Because of their diverse chemical and physical properties, the zircon structure-types are of interest to a wide variety of fields and may be used in geochronology, and as ceramic nuclear waste forms and aeronautical environmental barrier coating. To support advancement of their applications in geochemistry and materials development, 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 endmembers (i.e., zircon ($ZrSiO_4$), xenotime (YPO_4)), and monazite and xenotime solid solutions. Specifically, we provide an overview of 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. We hope this up-to-date summary of knowledge of zircon-type materials will help geochemists and materials scientists to continue developing fundamental understanding in mineralogy and geochemistry and promoting the use of zircon-type materials for applications, such as actinide waste forms and for aeronautical engineering as environmental barrier coatings.