Surface thermodynamics of yttrium titanate pyrochlore materials

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Pyrochlore-based ceramic waste form (A2B2O7) is one of the promising candidates for immobilizing long-lived isotopes from high level nuclear waste. While pyrochlore materials have been heavily investigated in the bulk size for thermodynamic stability and radiation resistance, relatively limited work has been performed at the nanoscale. The main difference is that enthalpy contributions from interfaces and surfaces are negligible in the bulk phase, but may greatly influence the thermodynamic stability of nanoparticles. Thus, in this work, we are extracting surface energy of a series of nanosized yttrium titanite pyrochlores from experiments, including high temperature drop solution oxide melt calorimetry (for enthalpy of formation), X-ray diffraction, and Brunauer-Emmett-Teller analysis (for crystalline and grain sizes).