

Studying oxides, alloys, gas hydrates, borohydrides, and metal-organic-framework structures using the Rietveld method

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Over the last several years we have been using the Rietveld method to understand the atomic structure of a wide variety of materials including $Ba_4Nb_2O_9$, biologically synthesized Fe_3O_4 , $(TeGe)_{0.85}-(AgSbTe_2)_{0.15}$ (TAGS85), Ti_4AlN_3 , $Mo_5Si_3-V_5Si_3$, gas hydrates containing the guest molecules CO_2 , CH_4 , C_2H_6 , and C_3H_8 , and we are beginning studies of borohydrides and metal-organic- and metal-porphyrin-framework structures. For some of the oxides, alloys, and gas hydrates we have studied the materials as a function of temperature and from refined lattice parameters we have calculated the thermal lattice expansion. For the Mo_5Si_3 we were able to reduce the high thermal expansion anisotropy by finding an optimum $(Mo_{1-x}V_x)_5Si_3$ composition and locate within the structure the site where the V atoms preferred to substitute. The refinements of the $Mo_5Si_3-V_5Si_3$ structures were improved by using soft constraints to keep the composition within a reasonable range of the nominal composition. For the TAGS85 and gas hydrate studies we tracked the atomic displacement parameters as a function of temperature to understand disorder within the structure. The studies of the gas hydrates necessitated the use of rigid bodies to describe the gas molecule disorder and we have started to employ time/temperature dependent studies to track the decomposition of the gas hydrate structure to ice.

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