SYSTEMATIC NEUTRON SCATTERING INVESTIGATION OF STRUCTURAL EVOLUTION IN PYROCHLORES AT LOW AND HIGH TEMPERATURES

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Pyrochlore structures $R_2Ti_2O_7$ (with R being a rare earth element) belong to the $Fd\bar{3}m$ space group and the family of rare earth titanates. Recently, pyrochlores have attracted great attention as nuclear waste form and possible high temperature solid oxide fuel cell (SOFC) materials. Furthermore, $Dy_2Ti_2O_7$ was reported by several authors to be the first structure in which magnetic monopoles were observed. This latter observation is related to the existence of spin ice in these structures, a phenomenon referring to a geometrical frustrated magnetic system, whereby "frustration" describes the effects that occur when interactions of similar strength compete and prevent a system from settling into a unique ground state. In spin ices, like $Dy_2Ti_2O_7$, only the rare-earth atoms have a magnetic moment and these cations reside in a network of corner sharing tetrahedra forming the pyrochlore lattice.

Neutron diffraction is a uniquely capable probe for these materials since both cation and oxygen anions as well as the magnetic structure can be investigated. Here we present structural parameters such as cation ordering, bond lengths and bond angles to quantify the geometrical frustration and characterize the crystal structure over a temperature range from ~5K to 1300K. The lower end of this range is of great interest to the solid state physics community and focuses on the geometric frustration leading to the formation of magnetic monopoles, whereas the characterization in the high temperature range will be of great use for the development of this material class as nuclear waste forms and solid oxide fuel cell materials.