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Atomic Motion in Crystals from Neutron Diffraction Experiments

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Static or dynamic disorder in crystals causes a decrease in the Bragg peak intensity, and given sufficient number of Bragg peaks over an extended Q-range, atomic displacement parameters (ADPs) can be refined that quantify the intensity reduction due to the mean square displacements of atoms about their average positions. It is becoming increasingly apparent that ADPs constitute equally important structural information as atom positions and site occupancies. Unusual, yet accurately determined, ADPs can provide telltale clues to interesting physical phenomena, e.g., approach of phase transitions, glass-like thermal conductivity, pathways for high ionic conductivity, and a variety positional disorders. Consequently, the demand for high quality ADPs is increasing, owing in part to our desire to understand and tune physical properties of technological materials. Temperature dependent neutron diffraction using single-crystals is perhaps the best possible method to determine precise individual ADPs, yet the number of these studies is surprisingly limited owing to the paucity of neutron sources and dedicated single-crystal neutron diffractometers. ADPs exhibit various temperature dependent behaviors, and can range from harmonic to anharmonic. Examples from work completed and ongoing at Oak Ridge National Laboratory (stephanite, triphylite, amblygonite, petalite, brucite, filled-skutterudites, gas clathrate hydrates, etc.) as well as previously published work will be reviewed with the aim to generalize insights and recommendations. Research conducted at ORNL's High Flux Isotope Reactor and Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

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