Optimizing the dynamic pair distribution function method for inelastic neutron spectrometry of polycrystalline Ni

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The Dynamic Pair Distribution Function (DyPDF) is an inelastic neutron scattering method that provides detailed information about the local dynamics of a crystalline material in real space. DyPDF has been applied to many systems, including ferroelectrics, superconductors, and charge density wave materials but a more complete adoption has been limited by lack of proper data treatment, understanding of the effects of different spectrometers, and a robust method of data analysis. In this work, we provide suggestions on optimizing the use of DyPDF based on case studies of polycrystalline nickel on several inelastic neutron scattering instruments including ARCS, MERLIN, and MARI. A robust data treatment regimen is outlined to enable quantitative comparison of data across spectrometers and an explanation and comparison of the instrumental effects are presented. We show that, by a careful choice of instrument and experimental conditions, DyPDF can serve as a routine real space complement to traditional local vibrational probes such as infrared and Raman spectroscopy.