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Simulated models of inhomogeneous broadening in perturbed angular correlation spectroscopy¹ JEFFERY A. HODGES, TYLER PARK, MICHAEL STUFFLEBEAM, W. EVENSON, P. MATHESON, Utah Valley University, M.O. ZACATE, Northern Kentucky University — All real crystals have defects such as impurities and vacancies which affect their properties. In perturbed angular correlation (PAC), these defects produce damping of the correlation signal in time and broadening of the frequency spectrum. This broadening is termed "inhomogeneous broadening" since it is due to the inhomogeneities (i.e. defects) in the crystal. We have simulated PAC spectra for various concentrations (0.1%) to 15%) of randomly distributed defects with a near-neighbor vacancy in simple cubic and face-centered cubic crystal structures. For every particular set of defects, the randomly distributed defects and the near-neighbor vacancy together produce a net electric field gradient (EFG), from which we obtain the PAC spectrum. We then average PAC spectra to study the effects of defect concentration and crystal structure on inhomogeneous broadening as an aid to analyzing experimental data. This work will be applied initially to broadened PAC data from β -Mn, Al-doped β -Mn, and Sr_2RuO_4 .

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