Abstract Submitted
for the 4CF07 Meeting of
The American Physical Society

Simulated models of inhomogeneous broadening in perturbed angular correlation spectroscopy (PAC)[1] MICHAEL A. STUFFLEBEAM, JEFFERY A. HODGES, WILLIAM E. EVENSON, P. MATHESON, Utah Valley State College, M.O. ZACATE, Northern Kentucky University — All real crystals have defects: missing atoms (vacancies), impurities, atoms out of place, etc. 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 5%) of distant randomly distributed defects plus 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 fit average PAC spectra to study the effects of defect concentration and crystal structure on inhomogeneous broadening as an aid to analyzing experimental data.

[1]Work supported in part by NSF grant DMR 06-06006 (Metals Program).

William Evenson
Utah Valley State College

Date submitted: 11 Sep 2007 Electronic form version 1.4