

Abstract Submitted
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Influences of small clusters of defects near probe nuclei in cubic structures in perturbed angular correlation models F. SULLIVAN, M. ADAMS, P. MATHESON, Utah Valley University, W.E. EVENSON, Retired — Evenson, et al. [1] have modeled concentration-dependent inhomogeneous broadening (IHB) in perturbed angular correlation (PAC) spectra for cubic structures by finding a suitable set of coordinates to represent electric field gradients (EFGs) and then characterizing their probability distribution functions (PDFs). For defect concentrations $c > 3\%$, a nonlinear transformation of the EFG components V_{zz} and V_{xx} produces two nearly-independent coordinates, W_1 and W_2 . Their PDFs are well characterized by gamma and alpha-stable distributions. These can then be used to reconstruct PAC spectra for arbitrary $c > 3\%$. However for $c < 3\%$, chance occupations by a small number of defects near the probe nucleus can distort the PDFs. For example, a single defect in shell two produces strong secondary peaks in the PDFs. Also, the joint PDF for $c < 3\%$ remains skewed, reflecting some influence of the crystal geometry. Parsing the PDFs by contributions from different arrangements of defects in near-probe shells, allows us to investigate the relative contributions of different defect configurations to the PAC spectrum. We report on progress made in modeling low defect concentration PDFs and their PAC spectra in SC, FCC and BCC structures.

[1] W.E. Evenson, M. Adams, A. Bunker, J. Hodges, P. Matheson, T. Park, M. Stufflebeam, M. O. Zacate, *Inhomogeneous broadening of PAC spectra with V_{zz} and η joint probability distribution functions*, Hyperfine Interact, 21 November, 2012

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