

Abstract Submitted  
for the 4CF12 Meeting of  
The American Physical Society

**Modified EFG Components and Their Joint pdf for Use in Modeling ihb in PAC** M. ADAMS, P. MATHESON, T. PARK, M. STUFFLEBEAM, J. HODGES, Utah Valley University, W.E. EVENSON, Retired, M.O. ZACATE, Northern Kentucky University — Spectra of hyperfine interactions involving the electric field gradient tensor (EFG) are subject to broadening by statistical variations of EFG components. In perturbed angular correlation (PAC) experiments, the inhomogeneous broadening (ihb) of the  $G_2(c,t)$  spectrum is produced by randomly distributed lattice defects of concentration,  $c$ . The EFG tensor has two independent components. The concentration dependence of ihb is determined by the joint probability distribution function (pdf) of these components. In typical PAC analyses, the independent coordinates are assumed to be  $V_{zz}$  and the asymmetry parameter  $\eta = (2V_{xx} + V_{zz})/V_{zz}$ . However, the pdf  $P(c, V_{zz}, \eta)$  is not known, and in any case it is easy to show that  $V_{zz}$  and  $\eta$  are highly correlated, and not independent. We have found that the application of the Czjzek transformation [1], followed by a simple conformal mapping produces two, nearly independent EFG coordinates  $W_1(c, V_{zz}, \eta)$  and  $W_2(c, V_{zz}, \eta)$ . The pdfs of each coordinate are readily characterized, and their product  $P(c, W_1, W_2) = P_1(c, W_1)P_2(c, W_2)$  forms an appropriate joint pdf that can be used to model ihb in a variety of situations. We show the application of this method by reporting results modeling the concentration dependence of ihb in various PAC models, for simple cubic (sc), face-centered cubic (fcc) and body-centered cubic (bcc) lattices.

[1] Czjzek, G. Hyperfine Interactions 14(1983) 189-194.

Philip Matheson  
Utah Valley University

Date submitted: 21 Sep 2012

Electronic form version 1.4