

Abstract Submitted
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Application of Polypacfit to obtain jump frequencies of probe atoms among sites having collinear EFG axes in Al_4Ba phases RANDAL NEWHOUSE, Washington State University, MATTHEW ZACATE, Northern Kentucky Univeristy, GARY S. COLLINS, Washinton State University — The Al_4Ba structure has two inequivalent Al-sites that have local electric field gradients (EFGs) collinear with a tetragonal crystal axis. Rapid diffusional jumps between the two sites leads to motional averaging of nuclear quadrupole interaction signals, as detected using perturbed angular correlation of gamma rays (PAC). However, unlike in the case of jumps that lead to reorientation of EFG axes and a loss of coherence of quadrupole precessions [1], motional averaging here leads to more subtle effects. A new program, Polypacfit, can be applied for fitting PAC spectra for nuclear relaxation to determine atomic jump frequencies in the Al sublattice. Polypacfit generates a PAC spectrum based on orientations of principal axes of the EFG specified by the user and fits this to experimental data. Polypacfit expands the range of systems in which PAC can be used to obtain diffusion data. *Supported in part by the NSF under grant DMR 09-04096 (Metals).*

[1] M.O. Zacate, A. Favrot and G.S. Collins, Phys. Rev. Lett. 92, 225901 (2004).

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