

PAC studies of diffusion using nuclear quadrupole relaxation

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One approach to the study of atom movement in solids is to measure an observable that is sensitive to discrete atomic jumps in real time. Such an observable is the electric field gradient (EFG) detected at the nucleus of a jumping tracer atom when the geometry of the diffusion sublattice is such that the EFG reorients in each jump [1]. Reorientation leads to a time-dependent attenuation of the static quadrupole interaction that can be fitted to obtain the jump frequency w .

We have investigated this type of quadrupole relaxation at nuclei of diffusing ^{111}Cd tracer atoms using perturbed angular correlation spectroscopy (PAC). Systems studied have the L1_2 (Cu_3Au) structure, including various In_3RE compounds, in which $\text{RE} = \text{La}$ [1], Ce, Pr, Nd, Er or Y, and Sn_3La . The Cu-type sublattice has three equivalent sites with tetragonal point symmetry and principal axes of the EFG aligned along cube directions. Each jump to a neighbouring site leads to reorientation of the EFG by 90° . Typical spectra for Sn_3La are shown in the figure. The nearly static perturbation function observed at 587 K becomes increasingly damped at higher temperatures due to diffusion, with the jump frequency proportional to the observed relaxation rate. Jump frequencies w were determined by fitting spectra directly with perturbation functions generated using the appropriate stochastic relaxation model.

I will summarize results obtained using this method and compare it with the conventional tracer diffusivity method. The tracer diffusivity D and w are related in cubic structures via $D = \frac{1}{12} f a^2 w$, in which a is the lattice parameter and f is the

correlation coefficient of diffusion. Thus, one can determine the correlation coefficient experimentally through a combination of diffusivity and jump-frequency measurements using the same tracer. It will be shown that the method is well suited for measuring jump frequencies at the boundary compositions of so-called “line” compounds which have narrow phase fields.

[1] Matthew Zacate, Aurélie Favrot and Gary S. Collins, *Physical Review Letters* (accepted).

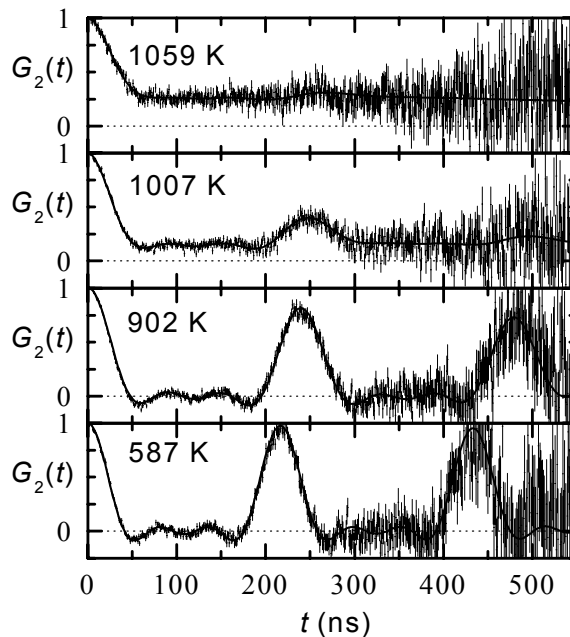


Figure 1: PAC spectra of Sn_3La at the indicated temperatures, exhibiting relaxation at high temperature attributed to diffusion.

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