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NUCLEAR SPIN RELAXATION

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Abstract

Nuclear spin relaxation rates due to magnetic dipole interactions and atomic diffusion in solids are calculated for some two- and three-dimensional systems and for some models of common diffusion mechanisms.

NMR magnetic dipolar spectral density functions are obtained for some lattice diffusion models for two-dimensional lattice diffusion on a square lattice and compared with the results for the BPP and continuum diffusion models. Numerical results and analytic approximations are obtained for dipolar interactions between spins diffusing in a plane, and interactions between diffusing spins in a plane with fixed spins in a separate parallel plane. Results for the longitudinal spin relaxation rates in the laboratory and rotating frames are obtained for square lattices and show strong dependence on the direction of the applied magnetic field relative to the crystal axes.

A simple matrix expression is derived for the atom jump probabilities due to an interstitial defect moving by an interstitialcy diffusion mechanism. This expression is used to obtain the tracer correlation factor and to calculate the atom jump probabilities numerically for various cubic and two-dimensional systems. An integral expression, involving atom jump probabilities, is obtained for the atomic displacement probabilities due to a single atom-defect encounter.

Expressions for the atomic displacement probabilities are used to calculate NMR magnetic dipole spectral density functions for atomic diffusion in LiF by the vacancy and interstitialcy diffusion mechanisms using the encounter model. Nuclear spin relaxation rates (R_1, $R_{1\rho}$ and R_2) of the F nuclei in LiF due to the diffusion of Li nuclei by these mechanisms are calculated from the spectral density functions and compared with the results of the BPP approximation. Measurements of the nuclear spin relaxation rates are shown to be ineffective at distinguishing between the diffusion mechanisms in this case, although the correct theory for the diffusion mechanism is required to interpret experimental results accurately. The differences $R_2 - R_{1\rho}$ and $R_{1\rho} - R_1$ are examined in the low-frequency limit and the encounter model results are found to be proportional to $(\omega_I \tau_e)^{3/2}$ while the BPP approximation results are proportional to $(\omega_I \tau_e)^3$.

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