SPIN-LATTICE RELAXATION AND ATOMIC MOTIONS IN LiF

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Spin-lattice relaxation times of the ^{7}Li spins in LiF have been investigated using pulsed NMR techniqes to determine the dominant mechanisms contributing to the normal high field relaxation, $1/T_1$, at laboratory fields of several kilogauss and also those contributing to the rotating frame relaxation, $1/T_{1\rho}$, corresponding to effectively low fields obtained by keeping the spins saturated. The experiments exhibit the very long intrinsic T_1 of LiF enabling one to achieve exceptional sensitivity to very dilute and very long correlation time interactions with defects and impurities and to study these interactions in the relatively low temperature region, $T<400°K$.

The most outstanding relaxation phenomena, and the one of principal interest in this work, is due to the motion of vacancies bound to divalent impurities; these effects are observed in $T_{1\rho}$ for temperatures greater than about 280°K and completely dominate $1/T_{1\rho}$ at temperatures greater than room temperature. The bound vacancy activation energy measured from the experiments is 0.43 eV, which is about 0.2 eV less than the activation energy of free vacancies. The mechanism dominating the relaxation at these temperatures is the fluctuating quadrupolar interaction between the vacancy and nearby spins.

A strong collision theory is developed to explain rotating frame quadrupolar relaxation in several different regimes of vacancy jump times, τ_v. The rf field dependence of $T_{1\rho}$ indicates that the τ_v's that we observe are long enough that the quadrupolar interactions suffer no motional narrowing effects but remain sufficiently short that nuclei experiencing a large quadrupole interaction are effectively thermally isolated from other nearby nuclei for a time long compared with τ_v.

The dominant relaxation mechanism from nitrogen temperature to room temperature in both the laboratory frame and rotating frame measurements appears to be the interactions of both the Li and F spins with fast relaxing paramagnetic centers whose concentrations are only a few ppm. The relaxation behavior due to this process is in agreement with the theory of Lowe and Tse when one properly includes both nuclear spin species.

Above room temperature, the T_1's in high field remain insensitive to the vacancy motion dominating $1/T_{1\rho}$, but they show some structure which is strongly temperature dependent though relatively small in magnitude. That this structure is sample dependent identifies its source as trace impurities, but the experimentally observed complexity precludes any easy identification or detailed interpretation.