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Nuclear magnetic resonance of ^{8}Li ions implanted in ZnO

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ZnO is a wide direct bandgap (3.4 eV) semiconductor with promising electronic properties potentially useful in room temperature optoelectronic and spintronic devices. It can be used as a dilute magnetic semiconductor by tuning intrinsic or extrinsic magnetic defects while ZnO also demonstrates many unique surface effects such as a photogenerated metallic state. Imperative to utilizing these unique properties is understanding and controlling point defects in its hexagonal wurtzite structure that may lead to stable hole doping. We implanted a low energy (20-25 keV) beam of hyperpolarized spin-2 8Li ions and used β-detected nuclear magnetic resonance (β-NMR) to understand the stability, structure, and magnetic state of Li defects in ZnO [Adelman et al., arXiv:2109.08637v1]. Closely related to μSR used to characterize isolated hydrogen impurities in ZnO, β-NMR allows complementary investigations of light isotope dopants in the ultradilute limit.

Using 8Li simultaneously as the defect and probe, distinct Li sites are detected by measuring the coupling of the nuclear electric quadrupole moment to the asymmetric electronic charge distribution surrounding the 8Li nucleus. From 7.6 to 400 K, we find ionized shallow donor interstitial Li is exceptionally stable, verifying its role in self-compensation of the acceptor (Zn) substitutional. Like the interstitial, the substitutional defect shows no resolved hyperfine field above 210 K, indicating it is a shallow acceptor. By pulsing the 8Li beam, the spin-lattice relaxation is measured and indicates above 300 K the onset of correlated local motion of interacting defects. This is supported by resonance spectra collected with a CW frequency comb that enhances the amplitude of well-resolved quadrupolar multiplets and confirms a site change transition from disordered interstitial Li to the substitutional. The quadrupole hyperfine interaction exhibiting a T3/2 temperature dependence typical of non-cubic metals is also discussed.

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