

15th International Conference on Muon Spin Rotation, Relaxation and Resonance



Contribution ID: 212 Contribution code: STD-4 / P-MON-31

Type: Oral

Nuclear magnetic resonance of ^8Li ions implanted in ZnO

Sunday, 28 August 2022 11:30 (15 minutes)

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 $T^{3/2}$ temperature dependence typical of non-cubic metals is also discussed.

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Session Classification: Student Day

Track Classification: Semiconductors