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Probing hydrogen sites and negative hyperfine parameter in semiconducting BaSi2 by muon spin rotation

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Hydrogen passivation of defects is commonly used to reduce defects in semiconductors such as GaAs, diamond, and Si. We recently found by experiment that atomic hydrogen is also very effective in significantly increasing a minority-carrier lifetime (> 10 μs) in BaSi2, one of the emerging materials for thin-film solar cell applications. This means that defects no longer act as recombination centers in BaSi2 after hydrogen passivation [1-2]. But three has been no experimental data about the hydrogen site in BaSi2. We employed muons to study the hydrogen state in single-crystalline BaSi2. Distinct neutral muonium state was identified in the high transverse-field measurements. From the temperature dependence, negative hyperfine parameters was suggested. From the angle-dependence of the hyperfine parameter in the magnetic fields applied in the a x b, b x c, and c x a planes, and comparison to the calculations based on density-functional theory (DFT), the hydrogen site in the BaSi2 crystal is proposed.
[1] Z. Xu et al., Phys. Rev. Mater. 3, 065403 (2019).
[2] X. Xu et al., J. Appl. Phys. 127, 233104 (2020).

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