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Magnetic structure refinement in the Mott insulator NiS_2

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We present muon spin spectroscopy (μSR) measurements on the antiferromagnetic Mott insulator NiS_2. This compound features two subsequent magnetic phase transitions around 38.9K and 29K associated with the opening of a Mott gap. From the the rotation dependence of transverse field μSR measurements (Fig. 1b) we confirm the magnetic space group 205.33 in the 38.9K to 29K phase, refined from neutron diffraction [1]. Using dipolar field calculations, we identify a candidate muon stopping site on a 24d Wyckoff position (blue site in Fig. 1b inset). We then calculate the muon stopping sites by using ab-initio density functional theory (DFT) and relaxing a supercell containing a single muon (i.e. hydrogen) impurity. Indeed the lowest energy muon site is found within 0.2 Angstrom of the experimentally determined one (red site in Fig. 1b inset). In addition, DFT predicts a second stopping site at an 8c Wyckoff position (green site in Fig. 1b inset), that can fully explain a small satellite frequency that we observe in the spectra. We then use the number of observed frequencies in the low temperature phase as a constraint to exclude magnetic order parameters inconsistent with our results.

[1] S. Yano, et al., Phys. Rev. B 93, 024409 (2016)

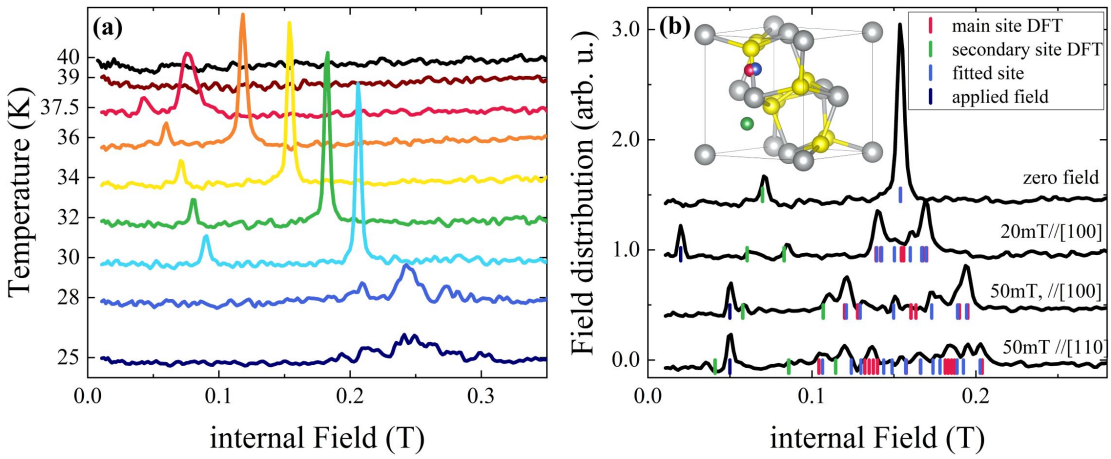

Figure 1: Local field distribution in (a) zero field and (b) transverse field. The curves are offset for clarity. The inset shows the candidate muon stopping sites.

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