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Evolution of the helimagnetic structure upon arsenic substitution for phosphorus in the Fe(P,As) system: NMR spectroscopy study

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Due to a series of nontrivial electronic, magnetic, and structural properties, transition metal pnictides with a MnP (B31) type structure have garnered significant interest in the scientific community. Helimagnetic ordering has been observed in the CrAs, FeAs, MnP, FeP compounds [1]. The recent discovery of superconductivity at high pressures in CrAs (Tc ~ 2.2 K at 1 GPa), MnP (Tc ~ 1 K at 8 GPa), and isostructural WP at ambient pressure with Tc ~ 0.7 K has sparked a new wave of research on B31 structure compounds.

Initial neutron powder diffraction studies of FeP and FeAs revealed an extremely unusual magnetic structure, which below TN = 120 K and TN = 77 K, respectively, consists of a combination of two helicoids [2, 3]. These incommensurate helicoids propagate along the crystallographic c-axis, with periods of ≈ 5 and 2.67 times the crystal lattice period in the Pnma representation. It was also reported that Fe ions possess weak magnetic moments of 0.4 μB in FeP and approximately 0.5 μB in FeAs. However, a recent comprehensive neutron scattering study [4] has demonstrated a more complex magnetic structure in FeAs, which is challenging to resolve using neutrons due to the low magnetic moment of Fe. For simplicity, the authors characterized the magnetic structure of FeAs as a noncollinear spin density wave (SDW) order with tilted moments in the ab plane. Mössbauer spectroscopy data indicates that the magnetic structure of FeP consists of a single strongly anharmonic helicoid with a temperature-independent anharmonicity parameter m = 0.9. Our NMR spectroscopy investigations on 31P nuclei, both for polycrystalline and single crystal samples, have revealed that the magnetic structure of FeP exhibits a doubled incommensurate helicoids [5, 6].

The present study aims to investigate the influence of isovalent substitution of arsenic for phosphorus on the magnetic structure of FeP. In this paper, we present measurements of 31P field-sweep NMR spectra at several fixed frequencies and zero-field NMR spectra at 4.2 K, performed on a single-phase polycrystalline FeP1-xAsx samples with x = 0.33 and 0.50. In contrast to the parent FeP compound, we observe a pronounced narrowing of the 31P NMR spectra, indicating a decrease in the induced magnetic field values on phosphorus. Moreove, the magnetic field profile on phosphorus is found to be Gaussian, likely indicating a decrease in the symmetry of the magnetic structure and a significant influence of fluctuations in FeP1-xAsx (x = 0.33, 0.50).

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