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Perturbed angular correlation study of the magnetic and structural first-order phase transition in MnAs

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text + references

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oral

Summary

The MnAs compound1 shows a first-order transition at ˜42 C, with structural (hexagonal-orthorhombic), magnetic (FM-PM) and electrical conductivity changes, and associated magnetocaloric, magnetoelastic and magnetoresistance effects. At ˜120 C it undergoes a second-order transition, becoming paramagnetic hexagonal. We report a study in the temperature range of -190-140 C, using the γ- γ Perturbed Angular Correlation method, complemented by first principles calculations.
The radioactive ion probe 77Se, with the double gamma decay cascade, implanted as 77Br, at ISOLDE-CERN laboratory is used to determine the Electric Field Gradient (EFG) and Magnetic Hyperfine Field (MHF) across the first-order phase transition encompassing the pure and mixed phase regimes in cooling and heating cycles. In the hexagonal phase the spectra is determined by the MHF whereas in the orthorhombic phase MHF is zero. The fractions of each phase are determined as a function of temperature. The temperature irreversibility of the first-order phase transition is seen locally, at the local atomic scale sensitivity of the hyperfine field, by the hysteresis of the fractions of each phase, in agreement with macroscopic magnetization and X-ray powder diffraction measurements. The MHF of the hexagonal phase is the same at a given temperature, irrespective of measuring on cooling or heating the sample, even in the phase coexistence region. The values of hyperfine parameters obtained using first-principles density functional theory with the LAPW method (Wien2k code2) are compared with the experimental results, considering the Se probe at both Mn and As sites, with the clear assignment of the probe location to the As sites.

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