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Program and abstracts
Magnetic spiral order in iron pnictides FeAs and FeSb

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Iron pnictides FeAs and FeSb exhibit very complex magnetic order pattern due to the competition between super-exchange covalent coupling and itinerant magnetism. Generally one observes anti-ferromagnetic order in the form of incommensurate planar spirals propagating along one of the crystallographic axes. There are two spirals differing by the shape of the spiral in the plane perpendicular to the propagation axis.

FeAs crystallizes within Pnma symmetry group. It was found that the spin spiral propagating along the c-axis leads to the complex variation of the hyperfine magnetic field amplitude with the spin orientation varying in the a-b plane. The magnitude of the hyperfine field pointing in the direction of the local magnetic moment depends on the orientation of this moment in the a-b plane. Patterns are vastly different for iron located in the [0 k 0] positions and for iron in the [0 k + ½ 0] positions within the orthorhombic cell. Lattice softens upon transition to the paramagnetic state at 69.2 K primarily in the a-c plane as seen by iron atoms. This effect is quite large considering lack of the structural transition. Two previously mentioned iron sites are discernible in the paramagnetic region till 300 K by different electron densities on the iron nuclei. The anisotropy of the iron vibrations developed at the transition to the paramagnetic state increases with the temperature in accordance with the harmonic approximation, albeit tends to saturation at high temperatures indicating gradual onset of the quasi-harmonic conditions [1]. Adjacent figures show unit cell of FeAs and spiral shapes.

The Fe₧₋₁Sb compound has been synthesized close to stoichiometry with x = 0.023(8). basically it conforms to the P6₃/mmc symmetry group with some interstitial iron present. The anti-ferromagnetic ordering temperature was found as 232 K i.e. much higher than for the less stoichiometric material. Regular iron was found to occupy two different
positions in proportion 2:1. They differ by the electric quadrupole coupling constants and both of them exhibit extremely anisotropic electric field gradient tensor (EFG) with the asymmetry parameter $\eta \approx 1$. The negative component of both EFGs is aligned with the $c$-axis of the hexagonal unit cell, while the positive component is aligned with the $<120>$ direction. Hence, a model describing deviation from the $P6_3/mmc$ symmetry group within Fe-planes has been proposed. Spectra in the magnetically ordered state could be explained by introduction of the incommensurate spin spirals propagating through the iron atoms in the direction of the $c$-axis with a complex pattern of the hyperfine magnetic fields distributed within $a$-$b$ plane. Hyperfine magnetic field pattern of spirals due to major regular iron is smoothed by the spin polarized itinerant electrons, while the minor regular iron exhibits hyperfine field pattern characteristic of the highly covalent bonds to the adjacent antimony atoms. The excess interstitial iron orders magnetically at the same temperature as the regular iron, and magnetic moments of these atoms are likely to form two-dimensional spin glass with moments lying in the $a$-$b$ plane. The upturn of the hyperfine field for minor regular iron and interstitial iron is observed below 80 K. Magneto-elastic effects are smaller than for FeAs, however the recoilless fraction increases significantly upon transition to the magnetically ordered state [2]. Figures below show unit cell of FeSb with the proposed deformation of the iron planes, magnetic spiral shapes and corresponding average hyperfine field distribution.

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References

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