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# First-order phase transitions in $CaFe_2As_2$ and phase separation in superconducting $Ba_{0.5}K_{0.5}Fe_2As_2$ and $Sr_{0.5}Na_{0.5}Fe_2As_2$ single crystals

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**Abstract** – $^{57}$Fe Mössbauer experiments in $Ba_{0.5}K_{0.5}Fe_2As_2$ and $Sr_{0.5}Na_{0.5}Fe_2As_2$ single crystals show the coexistence of a paramagnetic (superconducting phase) and a magnetic phase with strong static magnetic order. For the non superconducting $CaFe_2As_2$ a magnetic hyperfine field $B_{hf}$ was observed at the $^{57}$Fe nucleus below TN~170K indicating a first-order magnetic transition.

Recently, the ternary $A_{1-x}M_xFe_2As_2$ (A=Ca, Sr, Ba and Eu; M=K and Na) were found to shown similar structural, magnetic and superconducting properties with the related $RFeAsO_{1-x}F_x$ [1]. The $Ca_2Fe_2As$ undergoes a first-order high-temperature tetragonal to low-temperature orthorhombic phase transition at $T_S$~170K [2]. Concomitant with the structural transition the Fe moments order in a commensurate AFM structure [3]. This compound becomes superconducting either under moderate applied pressure and Na-doping [4,5]. The $Ba_{0.5}K_{0.5}Fe_2As_2$ and $Sr_{0.5}Na_{0.5}Fe_2As_2$ are superconductors with $T_c$ ~37 K and ~35 K, respectively. □ SR measurements have been shown a coexistence of superconductivity and phase separated static magnetic order in these compounds [6]. Mössbauer spectroscopy was used to investigate the magnetic and structural phase transition of single crystal $CaFe_2As_2$ as well the occurrence of phase separation in superconducting single crystals of $Ba_{0.5}K_{0.5}Fe_2As_2$ and $Sr_{0.5}Na_{0.5}Fe_2As_2$.

A mosaic of single crystal plates, with the *c* axes parallel to $\gamma$-ray direction, were used to perform the Mössbauer measurements. Room temperature measurements shown the main component of electric field gradient $V_{zz}$ is along *c* axis for these ternary compounds. For the non superconducting $CaFe_2As_2$ a magnetic hyperfine field $B_{hf}$ was observed at the $^{57}$Fe nucleus below $T_N$~170K indicating a first-order magnetic transition. Low temperature spectra fittings lead to $V_{zz}$ >0 with Fe moments lying in the (*a*,*b*) plane. The quadrupole splitting $\Delta E_Q$ values showed a discontinuity at ~170K showing that structural and magnetic transition occurs concomitantly. The Mössbauer spectra of $Ba_{0.5}K_{0.5}Fe_2As_2$ and $Sr_{0.5}Na_{0.5}Fe_2As_2$ shown a unique crystal site for Fe at room temperature however at 4.2K the presence of two phases is clearly observed. For $Ba_{0.5}K_{0.5}Fe_2As_2$ ~ 51% of Fe are in a paramagnetic state (superconducting phase) while the remaining are in a magnetic phase with small magnetic moments (~0.15$\mu B$). For $Sr_{0.5}Na_{0.5}Fe_2As_2$ only ~12% of Fe are paramagnetic, the remaining Fe are in a magnetic state with magnetic moments large as ~0.57$\mu B$. For $Sr_{0.5}Na_{0.5}Fe_2As_2$ only ~12% of Fe are paramagnetic, the remaining Fe are in a magnetic state with magnetic moments large as ~0.57$\mu B$.

## References

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