

Inelastic Neutron Scattering and Analysis of Magnetic Structure from powders of K doped and pure BaMn₂As₂ samples

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Low temperature powder inelastic neutron scattering measurements were performed on 3 different powder samples; parent BaMn₂As₂, 12.5 K doped Ba_{0.875}K_{0.125}Mn₂As₂ and 25 K doped Ba_{0.75}K_{0.25}Mn₂As₂. A magnetic model involving 3 different magnetic coupling constants; known as J1-J2-Jz Heisenberg Model, was used to define the scattering function. The corresponding intensities were calculated by a powder integration routine involving this Model using Monte Carlo integration methods. A series of magnetic intensities were calculated for different exchange constants. From these series, the best magnetic calculation was selected using a chi-square test yielding the magnetic exchange constant values.

The powder magnetic intensities were retrieved by subtracting the estimated background obtained from the non-magnetic high momentum transferred region from the raw data in the form of intensity versus transferred energy binned and averaged over all available momentum transferred range. The resultant estimated magnetic intensities were analyzed using a lineshape analysis which is modeled on a damped harmonic oscillator (DHO). The magnetic energy gap values obtained from DHO model is found to show an increasing pattern with the increase in the doped K amounts. The calculated energy gap values are also in agreement with the corresponding values which can be obtained visually from the S(q,E) scattering profiles. This is shown for Ba_{0.75}K_{0.25}Mn₂As₂ powder sample with 30 meV incident neutron beam energy data.

According to these analyses, a group of magnetic exchange constants were found to be the best values to define the magnetic scattering in these compounds. A representative set of 3 values were selected from these groups to define the pure and K doped BaMn₂As₂ magnetic exchange constant values. During the analysis, it was observed that the estimation for a background, mostly dominated with phonon scattering intensities along with other sources including the magnetic impurity scattering intensities for MnO becomes crucial in the comparison of the simulations with the raw data.

Over all, this is another conformation along with earlier studies using this technique that magnetic exchange constants can be calculated within an acceptable range with a very quick inelastic neutron powder experiment without a need for a single crystal sample.