Reconstruction of the Exchange Integrals Map of $M(FeAl)_{12}$ Incommensurate Structure

K. Rećko,[1] J. Waliszewski,[1] and K. Szymański[1]

[1] *Faculty of Physics, University of Białystok, Lipowa 41, 15-424 Białystok, Poland*

The compounds with the general formula $M(FeAl)_{12}$ (M = Ac, U, Re) crystallize in the body centered tetragonal symmetry. They form family showing a variety of magnetic structures, and in consequence of physical properties. The studies of (U, Th)$(FeAl)_{12}$ samples showed magnetic similarity in both series of actinide's systems. In the case of $Sc(FeAl)_{12}$ compound these rules turned out to fail. The magnetic structure is described by two modulation vectors: $k_1 = \{\varepsilon_x, \varepsilon_x, 0\}$ and $k_2 = \{-\varepsilon_x, \varepsilon_x, 0\}$, where respectively $\varepsilon_x = 9/50$ and $2/15$. In order to reconstruct the exchange integrals map reproducing the observed spin ordering, the atomic magnetic moments, modulation vectors and phase transition temperature the MCMag and MCPhase programs were used. Both of them are based on Kirkpatrick's algorithm simulates cooling or heating scenario, while the configuration space is examined by random sampling in accordance with the Metropolis procedure. However, two crucial aspects differ both methods. While MCPhase allows finding the exchange integrals out by fitting and treats the spins quantum-mechanically, so far MCMag treats the spins classically and the exchange constants have to be implemented and fixed.