Competition of ferromagnetism and superconductivity in Sc_3InB_x

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Recent discovery of superconductivity in the intermetallic perovskite $MgCNi_3$ was a great surprise due to large Ni contents and this compound was rather expected to be near ferromagnetic critical point. We present results of electronic structure calculations with Full–Potential KKR-LDA method for similar perovskite material – Sc_3InB – which is very promising candidate for a new superconductor. Interestingly, this compound may be regarded as a boron–inserted cubic Sc_3In, which is a high–pressure allotropic form of the well-known hexagonal weak ferromagnet Sc_3In. KKR calculations showed that scandium atoms keep magnetic moment (of about 0.25 μ_B) in both phases of Sc_3In, while Sc_3InB exhibits non–magnetic state with large DOS in the vicinity of E_F. Estimation of the electron–phonon coupling constant λ from McMillan–Hopfield formulas and calculated phonon DOS gave $\lambda \sim 1$ for Sc_3InB. The effect of vacancy in Sc_3InB_{1-x} and In/B disorder in Sc_3(In-B) on critical parameters were also discussed in view of KKR–CPA method. All theoretical results supported possibility of the superconductivity onset in Sc_3InB. A sample was prepared by arc melting technique and preliminary experimental data were collected using AC susceptometer equipped with a parallel resistivity measurement. The transition temperature was established close to 4.5 K, with a very abrupt change in susceptibility and a correlated drop of the resistivity when cooling down.

9.7 cm

13.4 cm

Subject category :

7. Computations of Electronic Structures

Presentation mode :

oral or poster

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