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Magnetic phase diagram of Mn(Ru-Rh)As - magnetoelastic and electronic properties

Dawid Szymański[1], Janusz Toboła[2], Ryszard Zach[3], Wiesław Chajec[3], Ryszard Duraj[3], Stanisław Baran[4], El Kebir Hlil[5], Daniel Fruchart[5]

[1]*Alpha Technology Sp.z.o.o sp. Komandytowa Ul. Balicka 182 30-149 Cracow, Cracow, Poland,* [2]*AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Al. Mickiewicza 30, 30-059 Cracow, Poland, Cracow, Poland,* [3]*Institute Of Physics, Cracow University Of Technology, Cracow, Poland,* [4]*Jagiellonian University Faculty of Physics, Astronomy and Applied Computer Science, Cracow, Poland,* [5]*Institut Néel CNRS -UGA, BP 166,, Grenoble, France*
E-mail: puzach@cyfronet.pl

The crystal structure of MnRu1-xRhxAs system belongs to the hexagonal Fe2P-type crystal structure (SG: P6 ̅2m). Mn atoms are located at pyramidal (3g) sites, Ru, Rh atoms at tetrahedral (3f) sites and As atoms occupy 1b and 2c positions. According to early works [1], for x < 0.24 and at low temperature the MnRu1-xRhxAs system exhibits ferromagnetic ordering with saturation magnetization of 3.96µB/f.u for x = 0. Increasing x(Rh) results in lowering Curie temperature. At low temperature, the MnRu1-xRhxAs system evidences a AF ordering for x > 0.24, while for x > 0.8 a complex (AF2+F) phase appears between the AF and the paramagnetic states. For x > 0.9 and below the complex (AF2+F) state a pure antiferromagnetic phase AF1 was found stable according to ref. [2].
Systematic XRD measurements were performed in the 80–550 K temperature range. The refinements of the crystal structure are reported here for x = 0, 0.1, 0.2, 0.3, 0.5, 0.8 and 0.95. From the thermal behavior of both the cell parameters and the atomic positions, an overall analysis of the magnetoelastic characteristics was established. It was found that the magnetic phase transitions are accompanied by jumps of cell parameters and volume. Furthermore in the presentation, detailed analysis of interatomic distances will be reported in details.
The MB(T) magnetization traces recorded in weak magnetic field allowed us to construct a novel (x,T) magnetic phase diagram for the studied solid solutions.
The investigations were devoted to the magnetocaloric effect (MCE) phenomena. Both positive and negative MCE have been observed and analyzed accordingly.
Besides, the interactions between the local magnetic moments and preferred type of magnetic ordering are analyzed as resulted from electronic band structure calculations performed using the Korringa-Kohn-Rostoker method in the coherent potential approximation (KKR-CPA).
For x = 0.2, 0.5, 0.95 the density of states (DOS) in (F) configuration exhibits a strong spin polarization arising mainly from a splitting of the Mn states. For MnRu0.8Rh0.2As and MnRu0.05Rh0.95As in (F) state the Fermi level is located near a DOS minimum of spin-up electrons density and near a small local maximum of spin-down ones. A somewhat different situation is observed for (F) MnRu0.5Rh0.5As: EF is located on a DOS minimum of spin-up electrons density and a large local maximum of spin-down ones. Moreover, the density of states decreases upon increasing x(Rh). In the case of (AF) MnRu0.8Rh0.2As, EF is located near a DOS maximum of spin-up and spin-down density. A similar situation is observed for (AF) MnRu0.5Rh0.5As where EF is located on a DOS maximum. For MnRu0.05Rh0.95As in (AF) state, EF is situated close to a DOS minimum for both of spin-up and spin-down density. Furthermore, for (AF) the density of states does not change with increasing rhodium. The results obtained from KKR method are in good agreement with those obtained from the neutron diffraction for parent compounds in terms of stability of the complex magnetic configurations

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