

Residual resistivity of (Ga,Mn)As alloys from ab initio calculations

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Abstract

The residual resistivity of diluted (Ga,Mn)As magnetic semiconductors with native compensating defects (As-antisites, Mn-interstitials) is calculated from first principles using the Kubo–Greenwood linear response theory. The concentration variations of the resistivity reflect the strength of impurity scattering and the number of carriers. In agreement with a recent experiment, the calculated resistivities are strongly correlated with the alloy Curie temperatures evaluated in terms of a classical Heisenberg Hamiltonian.

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The diluted magnetic semiconductors (DMS) attract interest because of their ferromagnetism mediated by the valence holes [1]. Whereas a number of first-principle studies address magnetic properties of the DMSs [2,3], existing theoretical investigations of their transport properties remain confined to a model level [4].

The p-type DMSs containing Mn atoms, such as (Ga,Mn)As alloys, are highly compensated systems due to native structural defects. The antisite As atoms [2,3] and the interstitial Mn atoms [5], both acting as double donors which add two electrons into the valence band, are the most probable compensating defects. Besides the chemical disorder, a new magnetic state stabilized by As-antisites and featured by a partial disorder in orientations of local Mn-magnetic moments has been predicted recently [3]. Here we report results of an ab initio study of the residual resistivity in (Ga,Mn)As alloys with the

native structural defects and the orientational magnetic disorder.

The electronic structure of the DMSs was determined in the local spin-density approximation using the all-electron scalar-relativistic tight-binding linear muffin-tin orbital method [6]. The substitutional disorder was treated in the coherent-potential approximation (CPA) [6] while the magnetic disorder was included within the disordered-local-moment (DLM) state [3,6]. The alloy residual resistivity ρ was evaluated in the Kubo–Greenwood linear-response formalism neglecting the CPA vertex corrections to the conductivity [7].

The calculated resistivities of the DMSs lie in the range $\rho \approx 0.5\text{--}5 \times 10^{-5} \Omega\text{m}$, i.e., in agreement with experiment [1,8] and an order of magnitude higher than those of metallic alloys [7].

The dependence of ρ on the concentration x of Mn atoms on the Ga-sublattice for two different concentrations y of As-antisites is shown in Fig. 1. In contrast to well-known trends for metallic alloys, the resistivity of the DMS decreases with increasing Mn-content. This behavior reflects two competing mechanisms: (i) the

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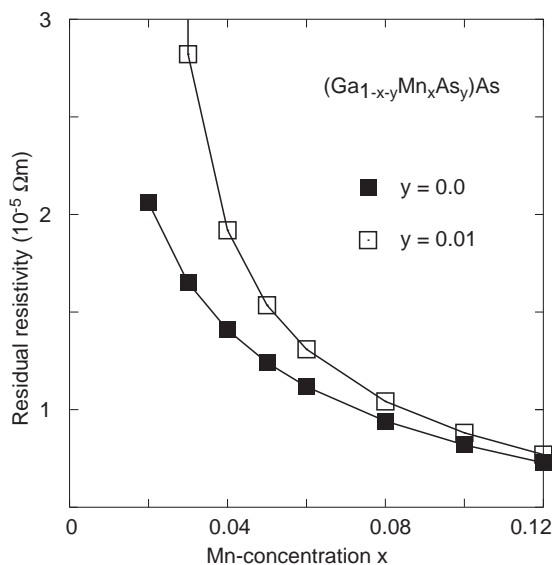


Fig. 1. Residual resistivity of (Ga,Mn)As as a function of the Mn-content: without As-antisites (■) and with 1% As-antisites (□).

increase of ρ with increasing concentration of impurities which is due to impurity scatterings, and (ii) the increase of the conductivity (the decrease of ρ) with increasing number of carriers which is proportional to the Mn-content. The latter mechanism is strong especially for compositions close to the full compensation ($x = 0.02$ for $y = 0.01$).

The other trends of ρ are less surprising: ρ increases with increasing concentrations of both As-antisites (Fig. 1) and Mn-interstitials, which is due to a superposition of the two above mechanisms. Results for alloys with local Mn-moments in the ferromagnetic state and in the DLM state (the ground state for non-negligible concentrations of As-antisites [3]) witness that the magnetic disorder leads to higher values of ρ .

Resistivity measurements have been used in a recent attempt to increase the Curie temperature T_C of (Ga,Mn)As thin films [8]. Fig. 2 shows the experimentally observed correlation between the conductivity (at 4.2 K) and the T_C for films with 5% Mn and the corresponding theoretical correlation obtained for $(\text{Ga}_{0.95-y}\text{Mn}_{0.05}\text{As}_y)\text{As}$ alloys ($0 \leq y < 0.025$). The alloy T_C 's were calculated using a classical Heisenberg

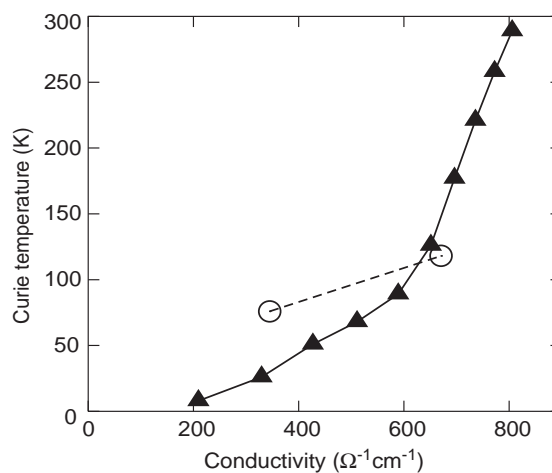


Fig. 2. The Curie temperature vs. the conductivity for (Ga,Mn)As with 5% Mn: calculated (▲) and experimental [8] (○).

Hamiltonian [9,10]. The semiquantitative agreement of the two correlations (Fig. 2) proves a strong dependence of both quantities on the degree of compensation (number of holes) present in this DMS.

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References

- [1] H. Ohno, J. Magn. Magn. Mater. 200 (1999) 110.
- [2] H. Akai, Phys. Rev. Lett. 81 (1998) 3002.
- [3] P.A. Korzhavyi, et al., Phys. Rev. Lett. 88 (2002) 187202.
- [4] T. Jungwirth, Q. Niu, A.H. MacDonald, Phys. Rev. Lett. 88 (2002) 207208.
- [5] F. Máca, J. Mašek, Phys. Rev. B 65 (2002) 235209.
- [6] I. Turek, et al., Electronic Structure of Disordered Alloys, Surfaces and Interfaces, Kluwer, Boston, 1997.
- [7] I. Turek, et al., Phys. Rev. B 65 (2002) 125101.
- [8] K.W. Edmonds, et al., Appl. Phys. Lett. 81 (2002) 4991.
- [9] M. Pajda, et al., Phys. Rev. B 64 (2001) 174402.
- [10] I. Turek, et al., Phys. Stat. Sol. B 236 (2003) 318.