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Magnetic properties of half-metallic semi Heusler $Co_{1-x}Cu_xMnSb$ compounds

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Abstract

A study of the half-metallic character of the semi Heusler alloys $Co_{1-x}Cu_xMnSb$ ($0 \leqslant x \leqslant 0.9$) is presented. We investigated the saturation magnetization M_S at temperatures from 5 K to room temperature and the temperature dependence of the DC magnetic susceptibility χ above Curie temperature T_C. The magnetic moments at 5 K, for most compositions are very close to the quantized value of 4 μ_B for Mn^{3+} ion, the compound with 90% Co substituted by Cu is still ferromagnetic with M_S (5 K) = 3.78 μ_B/f.u. These results emphasize the role of Co atoms in maintaining the ferromagnetic order in the material. The Curie temperature is decreased from 476 K to about 300 K as the Cu content increases from 0% to 90%. Above T_C, the χ^{-1} vs T curves follow very well the Curie–Weiss law. The effective moment μ_{eff} and paramagnetic Curie temperature θ are derived. A comparison between the values of M_S at 5 K and μ_{eff} shows a transition from localized to itinerant spin system in these compounds.

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1. Introduction

Ternary semi Heusler alloys XMnSb (X = 3d, 4d or 5d) which have $C1_b$ cubic structure (space group F-43 m) are ferromagnets with Curie temperature between 500 and 700 K except for CuMnSb which orders antiferromagnetically below 55 K [1,2]. Due to the high T_C and predicted half-metallicity, these alloys attract increasing interest in the field of spintronics. Half-metallic ferromagnets are characterized by the coexistence of metallic behavior for one direction of electron spin and insulating or semiconducting behavior (energy band-gap) for the other. Therefore, the electron density of states is ideally 100% spin polarized at the Fermi level and conductivity is governed entirely by single spin electron carriers [3,4]. The magnetic properties of half-metallic ferromagnets are manifested by quantization of the magnetic moment at 0 K and a change of spin system from localized to itinerant behavior upon increasing temperature [5]. Recently, by employing electronic band structure calculations, Galanakis et al. [6] have shown that CoMnSb has the largest spin-minority gap (~1 eV) among the XMnSb compounds, this gap is about 0.5 eV in the case of NiMnSb. The Fermi level in CoMnSb locates at the lower edge of the gap. A change of the lattice parameter by 2% still preserves the gap and shifts the Fermi level toward the lower edge and the higher edge as increasing or decreasing the lattice constant, respectively. In addition, the hybridization between the wave functions of 3d electrons of Co and Mn is considerably larger than that in the case between Ni and Mn. As a consequence, the Mn moment is reduced, while the Co moment becomes negative, resulting finally in a calculated total moment of 3 μ_B [6].

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In order to clarify the half-metallic character in CoMnSb, this paper deals with the magnetic properties of the $Co_{1-x}Cu_xMnSb$ series. Replacing Co by Cu, which is slightly larger than Co, will not affect the crystallographic structure but the band filling and hybridization.

2. Experimental

The polycrystalline $Co_{1-x}Cu_xMnSb$ samples ($0 \leqslant x \leqslant 1$, step 0.1) were prepared by arc-melting the constituent elements of 99.9% purity according to the stoichiometric formulae in a cold copper crucible and protective argon atmosphere. To compensate for evaporation losses, an excess of 5 wt% of Mn and Sb was added to the starting compositions. The molten ingots were heat treated at 1050 K in vacuum for 5 days and quenched in water in order to obtain good homogeneity. Crystal structure and microstructure analysis were carried out by means of X-ray diffraction (XRD) with Cu-K_α radiation and scanning electron microscopy (SEM), respectively. Magnetization at temperatures between 100 and 800 K is measured using a vibrating sample magnetometer in applied magnetic fields up to 1.4 T. For magnetization measurements at 5 K we employ a commercial SQUID magnetometer MPMS5S with maximal applied field of 5 T.

3. Results and discussion

All $Co_{1-x}Cu_xMnSb$ samples are characterized by XRD measurements. As typical examples, Fig. 1 shows the diagrams of compositions $x = 0$, 0.9 and 1. All the samples form in the cubic phase with space group $C1_b$. The development of the lattice parameter with variation of x is depicted in Fig. 2. A continuous expansion of the lattice occurs when x increases because the radius of a Cu ion (1.28 Å) is slightly larger than that of a Co ion (1.25 Å). The total change in lattice parameter is about 3.8% when x increases from 0 to 1.

The magnetization curves for the $Co_{1-x}Cu_xMnSb$ compounds at 5 K are shown in Fig. 3. The concentration dependence of the saturation magnetization M_S is plotted in Fig. 4. The values of the magnetic moments per formula unit are slightly larger than $4\,\mu_B$/f.u. for $x \leqslant 0.7$. The maximum value of $4.25\,\mu_B$/f.u. is observed for $x = 0.1$ and 0.2. This very small excess has also been reported in pervious works for CoMnSb, which can be attributed to a small contribution from Co moments [5,7,8]. The ferromagnetic ordering in the material is preserved with Cu substitution up to $x = 0.9$, with a still quite large $M_S = 3.78\,\mu_B$/f.u. and T_C near room temperature. These results indicate that in this series the magnetic moments are mainly localized on the Mn atoms. The variation of M_S at 4.5 K as a function of Cu substitution x for $Ni_{1-x}Cu_xMnSb$ alloys was recently investigated by Ren et al. [9]. They show that, for x lower than 0.7, the magnetic moments of the $Ni_{1-x}Cu_xMnSb$ compounds remain almost unchanged. However, when x is larger than 0.7, the values of the formula moments start to drop significantly, showing a breaking of ferromagnetic order. As already known, in semi Heusler alloys, the magnetic ordering is governed by the Mn–Mn interaction which proceeds via itinerant

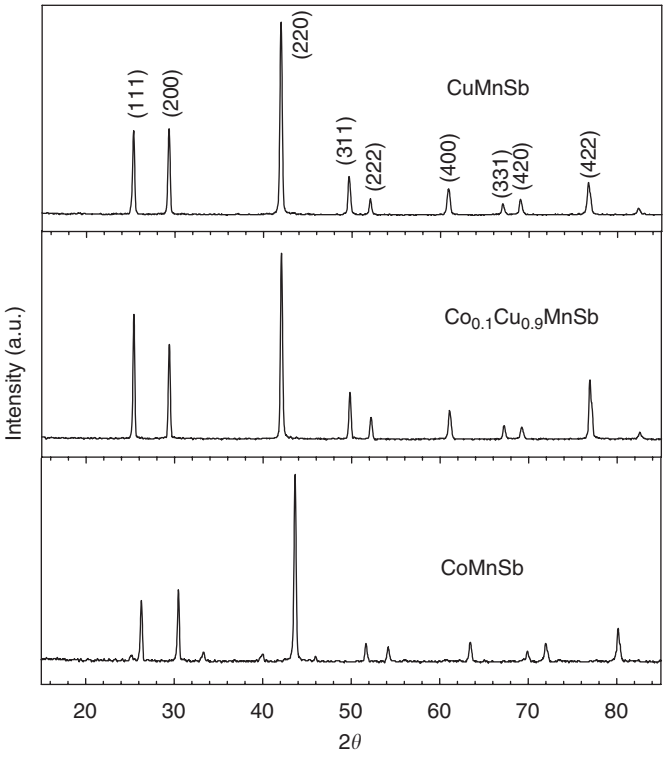

Fig. 1. X-ray diffraction spectra of the $Co_{1-x}Cu_xMnSb$ compounds ($x = 0$, 0.9 and 1).

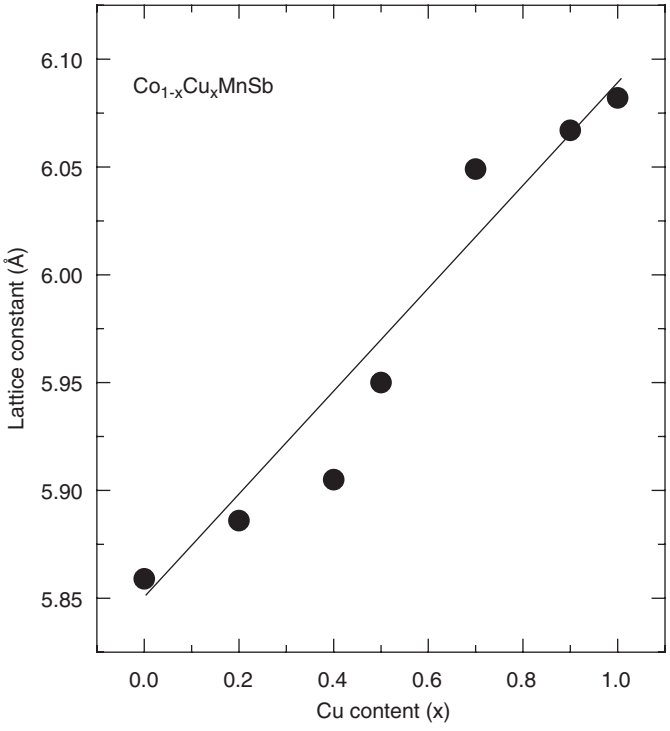

Fig. 2. Lattice constant of the $Co_{1-x}Cu_xMnSb$ compounds as a function of Cu substitution.