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Research articles

Structures, magnetism and transport properties of the potential spin-gapless semiconductor CoFeMnSi alloy

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ABSTRACT

The polycrystalline CoFeMnSi alloy with a potential spin gapless semiconductor (SGS) behavior was prepared by arc melting. The structures, magnetism and transport properties of CoFeMnSi alloy were investigated in detail. The occurrence of (1 1 1) superlattice XRD peak indicates the highly ordered Y-type structure of CoFeMnSi alloy. The saturation magnetization is around 3.49 μ_B/f.u. and the Curie temperature is about 763 K. The transport properties exhibit a semiconducting-like behavior and the resistivity is about 269 μΩ cm at 300 K. The carrier concentration almost shows a non-dependence of temperature, which is different from that of traditional semiconductor, presenting a typical characteristic of spin gapless semiconductor. The carrier concentration and carrier mobility measured at 300 K are 4.9×10^{20} cm^{-3} and 46 cm^2/V.s, respectively.

1. Introduction

Nowadays, Heusler-type spin gapless semiconductors (SGS) have received considerable interest in the fields of condensed matter physics and materials science due to their potential application in novel spintronic devices due to their specific band structure: top of the valence band and the bottom of the conduction band for the majority electrons touched at the Fermi level (E_F) with zero band gap, while a band gap observed for the minority electrons [1]. This special band structure of SGS can give rise to the following unique transport properties [2]: (1) the excitation of carriers with spin polarization of 100%; (2) no energy required to excite electrons from the valence band to the conduction band; (3) the completely separated polarized spin carriers based on Hall effect; (4) the ability to switch between spin-polarized carriers of *n*-type and *p*-type by applying a gate voltage; (5) carrier mobility is 2–4 times higher than that of conventional semiconductor because the modulation of the Fermi level could significantly change the concentration of spin-up and spin-down streams in the SGS; (6) the high sensitivity of SGS characteristics to external influences (e.g. temperature, electric field, stress, electromagnetic radiation and impurities), which are expected to be favorable to design the future spintronic devices [3].

Equiatomic quaternary Heusler compound CoFeMnSi alloy can be regarded as the intermediate product of Co_2MnSi [4] and Fe_2MnSi [5], which possess both half-metallic ferromagnetism and gapless semiconductor properties. CoFeMnSi alloy was originally considered to be a half-metallic ferromagnetic material [6–8] until its SGS behavior was found and proved in the theoretical and experimental studies [9–11]. Moreover, CoFeMnSi alloy is expected to be one of the potential substitutes for diluted magnetic semiconductors owing to its high Curie temperature (T_c) [12]. In addition, CoFeMnSi alloy is useful for counteracting resistivity mismatch with conventional semiconductors [13]. But there are few works to investigate its phase transformation, microstructure and transport properties under the solidification process. In this paper, we fabricated the CoFeMnSi alloy by arc melting and comprehensively studied its essential attributes, including structures, magnetism and transport properties. The results provide an important experimental evidence for the potential application of CoFeMnSi alloy in spintronic devices.

2. Experimental

Polycrystalline CoFeMnSi alloy was prepared by arc melting appropriate quantities of various elements (the purity is higher than 99.9%). Additional 5 wt% manganese was added to compensate for evaporation loss. The structure of the samples was characterized by x-ray diffraction (XRD, Shimadzu Limited) with Cu Kα radiation. The elemental composition was confirmed using scanning electron microscope (SEM, JEOL JSM-6700F). The high temperature magnetism was checked with vibrating sample magnetometer (VSM, 7035 model). The low temperature magnetism and transport measurements were performed within the temperature range of 5–300 K under an external magnetic field up to 30 kOe, using the Versa-lab comprehensive

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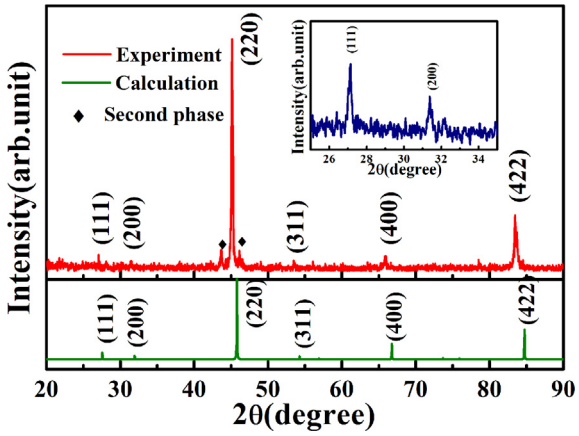

Fig. 1. Room-temperature X-ray diffraction pattern of CoFeMnSi compound and (inset) the expended part of the low angle region for XRD pattern.

physical analyzer (Quantum Design) and physical property measurement system (PPMS, Quantum Design PPMS-9).

3. Results and discussion

3.1. Structural properties

The ordering of Heusler alloys is directly related to the spin polarization, magnetism and transport properties [14]. Fig. 1 shows the room-temperature XRD pattern of CoFeMnSi alloy. It is reported from theoretical calculation that the LiMgPdSn-type equiatomic quaternary Heusler alloy CoFeMnSi is the highly ordered intermetallic compound with the prototype of Y-type structure (space group is F-43 m (#216) with the atomic label $XX'YZ$) [10]. In the Wyckoff coordinate, the structure can be defined as four interpenetrating fcc lattice and the face centered structures are arranged in a diagonal order of X-Y-X'-Z [10]. As seen from Fig. 1, the three typical diffraction peaks corresponding to CoFeMnSi (2 2 0), (4 0 0) and (4 2 2) can be observed, which indicate the polycrystalline structure of CoFeMnSi. From the expanded XRD pattern of the low angle region, as shown in the inset of Fig. 1, the diffraction peak of (1 1 1) can be observed, indicating the formation of highly ordered Y-type structure of CoFeMnSi [7]. To further estimate the chemical order of CoFeMnSi, we calculated the intensity ratios of I_{200}/I_{220} and I_{111}/I_{220}. It is reported that the superlattice reflections (2 0 0) and (1 1 1) are proportional to the chemical ordering factors defined as S^2 and $S^2\ (1-2\alpha)^2$, respectively [15]. And the two ordering factors can be described as:

$$S^2 = (I_{200}/I_{220})_{Exp.}/(I_{200}/I_{220})_{Theory} \quad (1)$$

$$S^2(1-2\alpha)^2 = (I_{111}/I_{220})_{Exp.}/(I_{111}/I_{220})_{Theory} \quad (2)$$

The $S = 0$ & $\alpha = 0$ and $S = 1$ & $\alpha = 0.5$ denote the disordered $A2$ structure and ordered $B2$ structure, respectively. The $S = 1$ and $\alpha = 0$ corresponds to the well-ordered cubic structure [7,15]. With respect to the XRD analyses, we calculated the $S = 1$ and $\alpha = 0$, demonstrating the CoFeMnSi in our work exhibiting a well-ordered cubic Heusler structure (LiMgPdSn-type or Y-type structure) [7]. In addition, the lattice constant of CoFeMnSi is 5.67 Å, which is 1.23% larger than the theoretical value (5.601 Å) [6].

The micro-morphology of the CoFeMnSi alloy is observed by SEM. As shows in Fig. 2(a), it is clear to see that there are three different regions (A, B and C regions) in the sample, implying that there exist three different phases in CoFeMnSi alloy. The average atomic concentrations as recorded by energy dispersive spectrum (EDS) spectroscopy for the A, B and C regions were $Co_{0.90}Fe_{0.95}Mn_{0.96}Si_1$, $Co_{0.99}Fe_{1.11}Mn_{1.59}Si_1$ and $Co_{0.81}Fe_{0.66}Mn_{1.21}Si_1$, respectively. According to the elemental mapping measurement (as shows in Fig. 2(b)),

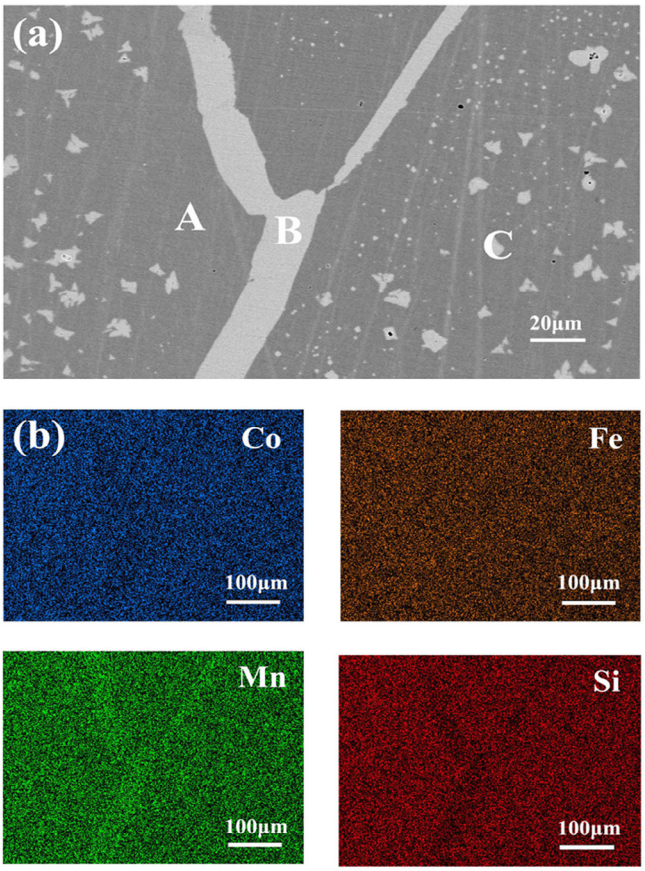

Fig. 2. (a) SEM image of the CoFeMnSi alloy at room temperature and (b) the elemental mappings of Co, Fe, Mn, Si, respectively.

the B, and C regions are Mn-rich phase, which could be corresponding to the impurity peaks in XRD pattern.

3.2. Magnetic properties

Fig. 3(a) shows the typical magnetic hysteresis loops measured at different temperatures for CoFeMnSi alloy. The inset of Fig. 3(a) presents the curve around the zero field for the measurement at 300 K. The sample is magnetically soft with extremely small coercivity as shown in the inset of Fig. 3(a). The saturation magnetization M_s is 98.6 emu/g (3.49 μ_B/f.u.) and smaller than the value of 4 μ_B/f.u. (mainly contributed by Mn atoms) based on the Slater-Pauling (SP) rule [12]. The discrepancy between experimental M_s value and the saturation moment predicated by SP rule is probably ascribed to the factors of presence of chemical disordered structures and impurities [12]. According to the XRD and EDS characterizations, the second phases, disordered structures and composition deviation of main phase can be observed in CoFeMnSi, which could give rise to non-integer position occupation or atomic site disorder. The dislocation of the Mn atoms could easily occur when Mn atoms and the neighboring Co or Fe atoms swapped or fell into tetrahedral space, leading to the decrease of total magnetic moment [8].

Fig. 3(b) shows the dependence of the spontaneous saturation magnetization (M_s) of the CoFeMnSi alloy on the temperature (T) and the inset is thermal magnetic curve. The curve can be well fitted by:

$$Ms(T) = cT^a + b \quad (3)$$

Here $a = 1.55$ and M_s (T) approximately follows the Bloch formula [16]:

$$M_s(T) = M_s(0)(1-kT^{1.5}) \quad (4)$$