

Electronic transport in Co-based half-metallic ferromagnetic Heusler alloys

V.V. Marchenkov¹, N.I. Kourov¹, K.A. Belozerova¹, S.M. Emelyanova¹, V.P. Dyakina¹, E.B. Marchenkova¹, M. Eisterer², H.W. Weber²

¹ Institute of Metal Physics, 620990 Ekaterinburg, Russia

² Atominstitut, Vienna University of Technology, 1020 Vienna, Austria

march@imp.uran.ru

Abstract. The electroresistivity of the Co-based half-metallic ferromagnetic Co₂CrGa, Co₂CrAl, Co₂VAl, Co₂MnAl Heusler alloys and the Ni₂MnGa ferromagnets were measured in the temperature range from 4.2 to 900 K. Specific features in the electrical resistivity of the half-metallic ferromagnetic Heusler alloys were observed, which can be explained in terms of the two-current conduction model, taking into account the existence of an energy gap in the electron spectrum near the Fermi level.

1. Introduction

The creation of a spin-polarized electron current and its control in conducting materials represent a promising trend in solid state physics. 100% spin-polarization can be realized in Heusler alloys, i.e. intermetallic X₂YZ compounds with the L₂₁ structure (X and Y are transition metals, and Z is an element from the III-V groups), which are being actively studied because of their possible application in spintronics. Band calculations performed for some Heusler alloys demonstrate the presence of an energy gap at the Fermi level in one of the spin subbands and a metallic type of electron states in the other subband. This peculiarity of the electron structure explains the term «half-metallic ferromagnets» (HMF) used for these alloys [1]. This feature of the electron spectrum, detected as a result of theoretical "ab initio" band calculations, is usually observed experimentally in the optical properties (see, e.g., [2-3]). Due to significant changes in the spectral parameters at the Fermi level, it should manifest itself also in other electronic properties, particularly, in the electronic transport. The purpose of this work is to study the effect of "gap" features in the electron energy spectrum near the Fermi level on the electrical resistivity of HMF Heusler alloys.

2. Experimental

We investigated the electrical properties of the Co-based HMF Co₂CrGa, Co₂CrAl, Co₂VAl, Co₂MnAl Heusler alloys as well as the ferromagnetic Ni₂MnGa compound. The alloys were prepared by arc melting in an argon atmosphere. The melted ingots were annealed at 1123 K for 24 hours in an argon atmosphere, followed by furnace cooling. The chemical composition was determined by energy-dispersive x-ray spectroscopy with an accuracy of $\pm 1\%$.

The structure analysis was performed by XRD investigations. The diffraction patterns were obtained at room temperature in a range of 2θ angles from 35° to 135° in steps of 0.02°. Monochromatic Cr-K _{α}



radiation with the wavelength $\lambda = 0.229$ nm was used. The analysis, carried out using the PowderCell program [4], shows that the Heusler alloys X_2YZ ($X = \text{Co}$; $Y = \text{Cr, V, Mn}$; $Z = \text{Ga, Al}$) have the structure $L2_1$, which contains eight bcc cells. The corners of each bcc cell, i.e. the 4a (0, 0, 0) and 4b (0.5, 0.5, 0.5) positions, are occupied by the X atoms, whereas the body-centered components, i.e. the 4c (0.25, 0.25, 0.25) and 4d (0.75, 0.75, 0.75) positions, are occupied by the Y and Z atoms, respectively [5]. The electrical resistivity was measured from 4.2 to 900 K by a conventional four-probe method.

3. Results and discussion

Figure 1 shows the temperature dependence of the resistivity $\rho(T)$ for the ferromagnetic Ni_2MnGa and the half-metallic ferromagnetic Co_2CrGa and Co_2CrAl Heusler alloys [6-8]. The magnitude of ρ and the form of the $\rho(T)$ dependence are significantly different. The residual resistivity (at $T = 4.2$ K) is $\rho_0 = 12 \mu\Omega\cdot\text{cm}$ in the ferromagnetic Ni_2MnGa alloy, $\rho_0 = 151 \mu\Omega\cdot\text{cm}$ and $\rho_0 = 128 \mu\Omega\cdot\text{cm}$ in the HMF Co_2CrAl and Co_2CrGa alloys, respectively. Furthermore, $\rho(T)$ in Ni_2MnGa shows a typical "metallic" behavior [9] with a positive temperature coefficient of the resistance (TCR), i.e. it increases with increasing temperature and has a kink near the Curie temperature T_C . The compound Ni_2MnGa undergoes a martensitic transformation near 200 K, which was not detected by resistance measurements, but manifested itself in the thermopower (see inset in Fig.1). In case of the HMF Co_2CrGa and Co_2CrAl alloys $\rho(T)$ shows a more complicated dependence with typical minima and maxima and temperature ranges with a negative TCR.

Table 1 lists the Curie temperatures, the HMF-state and the gap value for the Ni_2MnGa , Co_2CrGa and Co_2CrAl Heusler alloys. The Ni_2MnGa alloy is a typical ferromagnetic metal with no gap near the Fermi level. The other two, Co_2CrGa and Co_2CrAl , are half-metallic ferromagnets, which have an energy gap in the electronic spectrum for one spin subband (with spin down). The energy gap value is about 1 eV and 0.3 eV for Co_2CrGa and Co_2CrAl , respectively. Apparently, these features of the electronic band structure manifest themselves in the electrical properties.

Table 1. The Curie temperatures T_C , the HMF-state (HMF - half-metallic ferromagnets, FM - ferromagnet), and the values of the energy gap ΔE_F for the Ni_2MnGa , Co_2CrGa , Co_2CrAl , Co_2VAl and Co_2MnAl Heusler alloys.

Alloy	T_C (K)	HMF/FM	ΔE_F (eV)
Ni_2MnGa	390 [8]	FM	0 [10]
Co_2CrGa	495 [8]	HMF	1 [8]
Co_2CrAl	305 [6]	HMF	0.3 [7]
Co_2VAl	310	HMF	0.08 [11]
Co_2MnAl	697 [12]	near HMF	-

At temperatures below the gap temperature, there are two channels of conductivity in the HMF alloys: one for the electrons with spin up ($\uparrow$) and another for the electrons with spin down ($\downarrow$). The first channel of conductivity $\sigma_{\uparrow}$ has the usual form for ferromagnetic metals, i.e.

$$\sigma_{\uparrow} = \frac{1}{\rho_{\uparrow}}, \quad (1)$$

where

$$\rho_{\uparrow} = \rho_0 + \rho_{ee} + \rho_{ph} + \rho_m. \quad (2)$$

Here ρ_0 is the residual resistivity, ρ_{ee} , ρ_{ph} and ρ_m are the contributions to the total electroresistivity due to the electron-electron, electron-phonon and electron-magnon scattering, respectively.

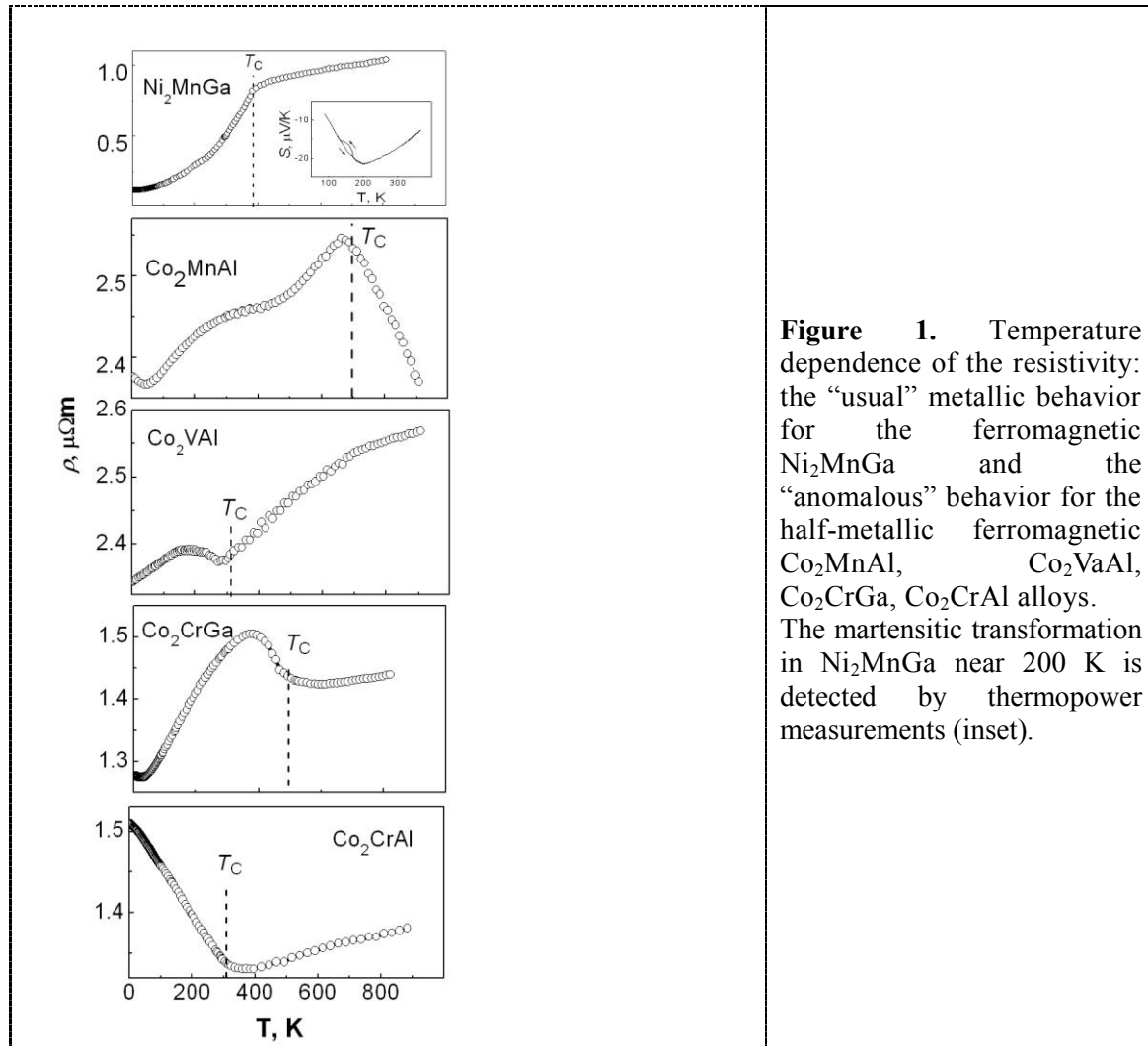


Figure 1. Temperature dependence of the resistivity: the “usual” metallic behavior for the ferromagnetic Ni_2MnGa and the “anomalous” behavior for the half-metallic ferromagnetic Co_2MnAl , Co_2VAl , Co_2CrGa , Co_2CrAl alloys. The martensitic transformation in Ni_2MnGa near 200 K is detected by thermopower measurements (inset).

The second channel of conductivity $\sigma_{\downarrow}$, for electrons with spin down, should strongly depend on the parameters of the energy gap in the electronic spectrum near the Fermi level. $\sigma_{\downarrow}$ should have either an exponential dependence, i.e., $\sigma_{\downarrow} \sim \exp(-T_0/T)$, where T_0 is the gap temperature, or a power dependence $\sigma_{\downarrow} \sim T^n$, where n is a power index. Since these two channels have a completely different temperature dependence, i.e. $\sigma_{\uparrow}$ decreases and $\sigma_{\downarrow}$ increases with T , the peculiarities of $\rho(T)$ ($\sigma(T)$), particularly the negative TCR, the extremes near T_C and the high resistivity value, can easily appear. Moreover a temperature dependence of the conductivity (resistivity) proportional to $\exp(-B/T^{1/4})$ (B is a coefficient) was observed in such high-resistivity alloys (see, e.g., Ref. [13]). This looks very similar to the Mott law “ $T^{1/4}$ ” [14], i.e. like the hopping conductivity with a variable hopping length. We assumed that the conductivity of the Heusler alloys can also be proportional to $\exp(-B/T^{1/4})$. To verify this assumption, the resistivity (conductivity) of the Co_2MeAl ($\text{Me} = \text{Cr}, \text{Mn}, \text{V}$) alloys was studied.

For the data analysis the concept of coexistence of elastic and inelastic electron scattering was used [13]. According to Ref. [13], the temperature dependence of the conductivity in the high-resistance alloys can be written as

$$\sigma = \sigma(0) + \sigma_{in} = \sigma(0) + A \cdot \exp(-B/T^{1/4}), \quad (3)$$

where A and B are coefficients, $\sigma(0)$ is the usual metallic conductivity due to the elastic scattering processes, and σ_{in} is the conductivity associated with the inelastic scattering of charge carriers. The conductivity $\sigma(0)$ includes the residual conductivity and the conductivity due to the electron-electron and electron-phonon interactions. It is assumed that $\sigma_{in} \gg \sigma(0)$.

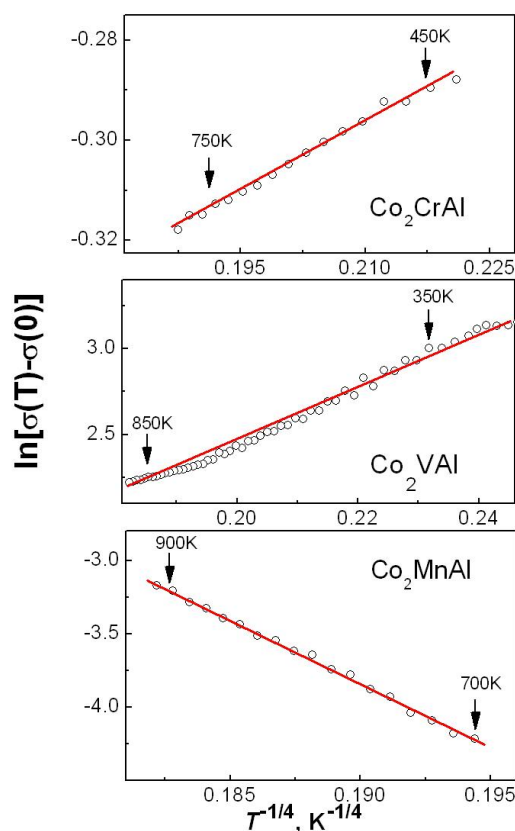


Figure 2. Dependence of $\ln[\sigma(T) - \sigma(0)]$ on $T^{-1/4}$ for Co_2CrAl , Co_2VAl and Co_2MnAl .

Fig. 2 presents the temperature dependence of the conductivity in the coordinates $\ln[\sigma(T) - \sigma(0)]$ versus $T^{-1/4}$ for the high-resistivity Co_2MeAl (Me = Cr, V, Mn) alloys. The conductivity follows $\sigma \sim A \cdot \exp(-B/T^{1/4})$ over a wide temperature range, which might also be a manifestation of peculiarities in the electron band structure near the Fermi level E_F of these alloys [8, 13]. Apparently, the sign of the coefficient B , and, hence, the type of the temperature dependence of the conductivity, can also be determined by features of the electron structure near E_F as well as by the relative contributions from different scattering mechanisms of current carriers to the total conductivity.

4. Conclusions

We demonstrated that the temperature dependence of the electrical resistivity in the half-metallic ferromagnetic Co-based Heusler alloys is predominantly determined by specific features of their band structure. The presence of an energy gap at the Fermi level E_F in one of the spin subbands of the conduction electrons with spin down can lead to anomalies in the resistivity, i.e. to a high residual resistivity, to extrema near the Curie temperature, and to a negative coefficient of resistivity. The conductivity is found to be proportional to $\exp(-B/T^{1/4})$ in these high-resistivity alloys at higher temperatures.

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