First principles study for the electronic structure and residual resistivity of Co$_2$MnZ (Z=Al, Si)

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Abstract. First principles calculations of electronic structure and electrical resistivity are performed for the bulk Co$_2$MnZ (Z=Al, Si) with the L$\bar{2}_1$, B2 and A2 structure respectively. The obtained result indicates that the L$\bar{2}_1$ and B2 structure are half-metallic and the degree of spin-polarization of the density of the states are close to 100%. However, half-metallicity is broken in the A2 structure and the degree of spin-polarization of the density of the states shows the opposite sign to those of L$\bar{2}_1$ and B2 structure. The residual resistivities due to the substitution type atomic disorder effect of the Co$_2$MnZ with the B2 and A2 structure are estimated in the order of 100 $\mu \Omega \text{cm}$, which are in good agreement with the experimental values at low temperatures.

1. Introduction
Heusler alloys are promising materials for a high degree of spin-polarization due to their half-metallicity. Recently, large tunnel magnetoresistance ratio has been reported in the magnetic tunnel junction using Co$_2$MnSi electrodes at low temperature [1, 2]. However, it is considered that the half-metallicity of the Heusler alloys would be sensitive to their crystal structures, and their half-metallicity are possibly broken by the variation of the electronic structure due to the lattice imperfection such as an atomic disorder or structural defects. There have been many works to calculate the electronic structures of Co-based Heusler alloys in first-principles [3, 4, 5, 6, 7], and these results indicate the suitable conditions that these alloys exhibit half-metallicity. On the other hand, the first principles study for the electrical transport property of Heusler alloys is so rare [8] that it is necessary to investigate these properties depending on atomic concentrations and crystal structures. The electrical resistivity of the Co$_2$MnSi with ordered structure is close to the values of 3d transition metal alloys around 10 $\mu \Omega \text{cm}$, while ones with disordered structure in the thin films are more than 100 $\mu \Omega \text{cm}$ by experimental measurements [9, 10, 11]. These facts imply that the transport property of Heusler alloys is also sensitive to their ordering. In the present work, we calculate the electronic structure and the electrical resistivity of the bulk Co$_2$MnAl$_{1-x}$Si$_x$ (x = 0.0, 0.2, ..., 1.0) and discuss about the relationship between the half-metallicity and transport property.

2. Calculation Methods
We consider three types of the atomic configuration of L$\bar{2}_1$ (ordered), B2 (Y-Z disordered) and A2 (X-Y-Z disordered) structures in X$_2$YZ (X=Co, Y=Mn, Z=Al, Si) as shown in Fig. 1. To
calculate the electronic structure, we employ the tight-binding linear muffin-tin orbital (TB-LMTO) method based on the local-spin density approximation (LSDA), and the substitution type atomic disorder effect in the B2 and A2 structure is treated by the coherent potential approximation (CPA) [12]. Note that we take $\delta = 0.5 \text{ mRy}$ as the infinitesimal damping constant to calculate the Green functions. The lattice constants of Co$_2$MnZ are set to the experimental values which is $a=5.755\text{Å}$ in Z=Al and $a=5.655\text{Å}$ in Z=Si [13]. In the intermediate region of $0.0 < x < 1.0$, the lattice constants depending on their concentration are determined by the Vegard law. The residual resistivity is evaluated by using the Kubo-Greenwood formula based on the method developed by Turek et al. [14]. About $10^6$ k-points are adopted to obtain more sufficient accuracy.

3. Results and Discussions

Figure 2 shows the density of the states (DOS) of the Co$_2$MnAl with the ordered L$_2^1$ structure and disordered B2 and A2 structure. In both L$_2^1$ and B2 structures, there is an energy gap at the Fermi level in the minority spin state, and these structures keep good half-metallicity. Therefore, a high degree of the spin polarization is expected from L$_2^1$ and B2 structure. However, the energy gap at the Fermi level is disappeared without a trace in the A2 structure and it goes to completely metallic regime. So we can consider that the half-metallicity of Heusler alloys is
Figure 3. Magnetic moments per Co$_2$MnAl$_{1-x}$Si$_x$ in the B2 and A2 structure as a function of Si concentration $x$.

Figure 4. Electrical resistivity of Co$_2$MnAl$_{1-x}$Si$_x$ in the B2 and A2 structure. The doubled circle is the experimental value at low temperature [11].

possibly influenced by the ordering of the Co-sublattice [3, 4, 5, 8].

Next, we look at the magnetic moments per Co$_2$MnAl$_{1-x}$Si$_x$ in the B2 and A2 structure in Fig. 3. When the total electron number is increased with $x$, the Fermi level is shifted to the higher energy side in Fig. 2. In the B2 structure, the moments in Fig. 3 are made greater in proportion to $x$, since the additional electrons occupy the majority spin state. As the result, the moments between $x = 0.0$ (Co$_2$MnAl) and $x = 1.0$ (Co$_2$MnSi) are increased from 4.0 $\mu_B$ to 5.0 $\mu_B$ as well as in the L2$_1$ structure [5]. On the other hand, these in the A2 structure are decreased with $x$, since its DOS in Fig. 2 of minority-spin state around the Fermi level is larger than that of majority-spin state.

Shown in Fig. 4 are the residual resistivities in the B2 and A2 structure. Note that these values of the resistivity include the extra contribution of the infinitesimal damping constant $\delta$ (=0.5 mRy) which increases the scattering probability in the system, so there may be some variation around 10 – 20% depending on the calculation condition. The obtained resistivities
are quantitatively corresponding to the experimental data at the low temperature [11]. In the B2 structure, the electrical resistivity tends to decrease with increasing of $x$ in spite of the decreasing of DOS of the majority spin state in Fig. 2, however, this tendency that the resistivity decreases with $x$ in the B2 structure is agreeable with the experimental measurement [15]. It is also remarkable that the electrical resistivity in the B2 structure is higher than that in the A2 structure. The total number of the electron states at the Fermi level in the A2 structure is larger than B2 structure, since the half-metallacity is broken in Fig. 2. The electrical resistivity is decreased by the contribution of the electrons of minority states, therefore, we can consider that the degree of spin-polarization of the electrical conductivity in the A2 structure becomes significant low or opposite sign to the L2$_1$ and B2 structure. In the future work, we would investigate this fact carefully in the view of the spin-resolved conductivity and more detailed studies are being carried out.

4. Summary
In this work, first principles calculations for the electronic structures and electrical resistivity of Co$_2$MnAl$_{1-x}$Si$_x$ ($x = 0.0, 0.2, ..., 1.0$) are performed by using the TB-LMTO-CPA method and Kubo-Greenwood formula. The present results show that Co$_2$MnAl$_{1-x}$Si$_x$ with the L2$_1$ and B2 structure keep good half-metallicity, although half-metallic gap is broken in the A2 structure. The residual resistivity due to subtitution atomic disorder effect is estimated in the order of $100 \mu \Omega \cdot cm$ in the B2 and A2 structure.

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