Electronic Structure and Magnetic Properties of Ni_2MnSn Heusler Alloy

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Abstract. The spin dependent momentum densities in Ni_2MnSn Heusler alloy have been measured at 10 and 300 K using magnetic Compton scattering. For these measurements, we have used 182.79 keV circularly polarized synchrotron radiation at SPring8, Japan. Spin dependent electron momentum densities are analyzed in terms of Mn 3d, Ni 3d and itinerant electrons to calculate their role in formation of net spin moment. Magnetic moments at different sites of constituent atoms have also been compared with the present full potential linearised augmented plane wave calculations and other available data.

Keywords: Synchrotron source X-ray scattering, Spin momentum density, Heusler alloys
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INTRODUCTION

Heusler alloys are very important due to their multifunctional properties such as magnetic super elasticity, gaint magnetoresistance, large inverse magnetocaloric effect and magnetic memory effect. These alloys are intermetallic compounds with stoichiometric composition X_2YZ having $L2_1$ type cubic structure in which X and Y are transition elements and Z is III, IV or V group element [1]. The interatomic exchange interactions and Curie temperatures in Ni_2MnX (X= Ga, In, Sn and Sb) are studied by Sasioğlu et al. using augmented spherical wave (ASW) method [2].

The magnetic Compton profile (MCP), $J_{mag}(p_z)$, is a projection of the spin dependent electron momentum densities along the scattering vector direction [3-4]. Mathematically, $J_{mag}(p_z)$ is written as

$$J_{mag}(p_z) = \iint \left[\rho^{up}(\mathbf{p}) - \rho^{down}(\mathbf{p}) \right] dp_x dp_y \qquad (1)$$

where $\rho^{up}\,\mathbf{p}$ and $\rho^{down}\,\mathbf{p}$ represent the electron momentum densities for the spin-up and spin-down electrons, respectively. The area under the MCP gives total spin moment (μ_{spin}) in μ_B/formula unit. The MCP is uniquely sensitive to the spin component of magnetic materials. In magnetic Compton scattering, we can also calculate the magnetic effect (R), which is ratio of intensities of charge Compton scattering to magnetic Compton scattering.

METHODOLOGY

The MCP measurements were carried out at the high energy inelastic scattering beam line BL08W at SPring-8 in Hyogo, Japan [4, 5]. Elliptically polarized synchrotron radiations (SR) of energy 182.79 keV were monochromatized by a bent Si (620) crystal. The peak brightness of SR from elliptical multipole wiggler was about 1.378 x 10^{17} phs^{-1} $mard^{-2}$ mm^{-2} per 0.1% bandwidth (BW) with critical energy of 42.6 keV. Energy distribution of Compton-scattered X-rays from the specimen were measured in back-scattering mode (178°) using a multi-segmented Ge solid-state detector with external magnetic field of 2.5 T and at different temperatures (10 and 300 K). The overall momentum resolution of spectrometer was 0.40 a.u. (Gaussian full width at half maximum).

The $J_{mag}(p_z)$ was deduced from the difference between two spectra with alternating directions of external magnetic field (switching time of 1 s). The

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raw spectra were corrected for the energy-dependent scattering cross-section, detector efficiency and sample absorption. The normalization (experimental magnetic moment) of the magnetic Compton profiles was determined using standard Fe sample.

On the theoretical side, we have used FP-LAPW method within local density approximation [6-7] to compute the magnetic moment of Ni_2MnSn alloy. To fulfill the convergence criteria, $R_{MT}K_{max}$, l_{max}, G_{max} and number of **k** points in the irreducible Brillouin zone were set to be 7, 10, 12 and 104, respectively.

RESULTS AND DISCUSSION

Fig. 1 shows the MCPs of the Ni_2MnSn alloy at 10 K, decomposed into individual components to obtain the splitted profiles whose sum was the best fit to the data. The area under each individual profile gives the magnetic moment at that site. The main contribution in the magnetic moment is due to the 3d electrons of Mn. Table 1 shows that the total experimental magnetic moment at 10 K is in reasonable agreement with theoretical magnetic moment calculated from FP-LAPW and available data. The total spin moment calculated at 300 K temperature was found to be 2.45 μ_B. The contribution of different components at 300 K, namely Mn 3d, Ni 3d (x2) and diffused was found to be 2.57, 0.28 and -0.62 μ_B, respectively.

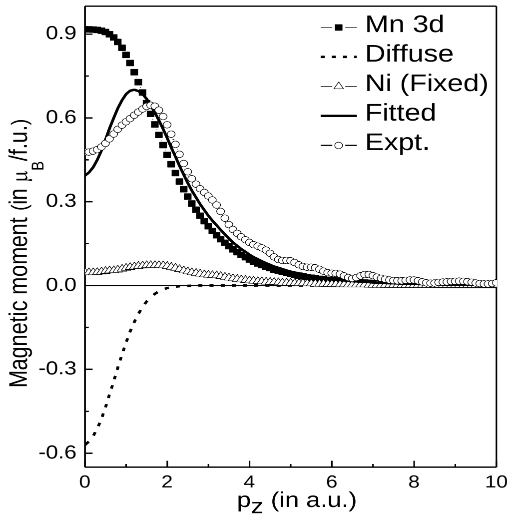

Figure 1. Spin polarized momentum distribution of Ni_2MnSn at 10 K decomposed into the Mn 3d, Ni (magnetic, fixed) and diffuse components. The best fit curve (fitted) in experimental MCP is a solid line passing through the experimental data points. Statistical error (±σ) in the experiment is within the size of the symbol.

TABLE 1. Spin magnetic moment of Ni_2MnSn using FP-LAPW scheme and experimental data. The error in the experimental spin moment is ±0.03 μ_B.

Method		**Spin Moment (μ_B)**	
		Site	**Total**
(i) Present work			
(a) FP-LAPW			3.93
	Ni x 2	0.44	
	Mn	3.48	
	Sn	-0.03	
	Intersitial	0.04	
(b) Experiment			4.05
	Ni x 2	0.44	
	Mn	4.26	
	Diffuse	-0.98	
(ii) Available data			
(a) FP-LAPW[1]			4.08
(a) ASW[2]			4.09

CONCLUSIONS

The magnetic Compton profiles of Ni_2MnSn at 10 and 300 K are reported. The MCPs have been analyzed in terms of Mn 3d and diffuse contributions. At low temperature (10K) the experimental spin moments deduced from the magnetic Compton profile are in good agreement with FP-LAPW calculations.

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