Study of magnetic moments of Fe₃Pt by X-ray magnetic diffraction

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Introduction

A ferromagnetic alloy Fe₃Pt shows the invar property that is thought to be related with magnetism. In this research we have measured spin and orbital magnetic form factor of Fe₃Pt separately by the X-ray magnetic diffraction (XMD) experiment and have obtained the spin and orbital magnetic moment by using atomic-model theoretical values for the form factors.

Experiment

The sample was a single crystal and was a sphere with a diameter 5mm. The crystalline structure is Cu_3Au -type in the order phase.

The XMD experiment has been performed on BL3C where the dedicated XMD experimental system is installed. We measured the spin and orbital magnetic form factor separately by utilizing the LS separation method. Here the spin and orbital magnetic form factor are denoted as $\mu_{\rm S}(K)$ and $\mu_{\rm L}(K)$ respectively, where $K=\sin\theta/\lambda$ (θ is Bragg angle, λ is X-ray wavelength).

Result and discussion

We have measured $\mu_S(K)$ and $\mu_L(K)$ for 26 and 21 reciprocal lattice points, respectively. The observed $\mu_S(K)$ and $\mu_L(K)$ are shown in Fig. 1 and Fig. 2. In these figures solid circles denotes the fundamental reflections the Miller indices (*hkl*) of which are all even or all odd, and open circles denote the superlattice reflections the Miller indices of which are mixed with even and odd integers.

In Fig. 1 it is noted that $\mu_{\rm S}(K)$ and $\mu_{\rm L}(K)$ of the superlattice reflections show different trends from those of the fundamental reflections due to the difference in the crystal structure factors for these reflections. In Fig. 2 it is shown that all $\mu_{\rm L}(K)$ values are close to zero which suggests that the orbital moment is almost quenched.

We estimated the spin and orbital magnetic moment of Fe and Pt by using atomic-model theoretical values for $\mu_S(K)$ and $\mu_L(K)$ under the dipole approximation. In this model $\mu_S(K)$ is presented as $\mu_S(K)=3m_{S,Fe}<j_{0,Fe}(K)>+m_{S,Pt}<j_{0,Pt}(K)>$ for fundamental reflections and $\mu_S(K)=m_{S,Pt}<j_{0,Pt}(K)>-m_{S,Fe}<j_{0,Fe}(K)>$ for superlattice reflections where $m_{S,Z}$ is spin magnetic moment of Z atom and $<j_{n,Z}(K)>$ is integral of radial wavefunction of Z atom multiplied by the n-th order spherical Bessel function. For $\mu_L(K)$ the above equations hold but $m_{S,Z}$ and $<j_{0,Z}(K)>$ are replaced with $m_{L,Z}$ and $<j_{0,Z}(K)>+<j_{2,Z}(K)>$. We used $<j_{n,Z}(K)>$ values for Fe and Pt in reference [1] and [2], respectively.

The least squares fitting analysis gave us the spin magnetic moment $1.99\pm0.01\mu_B$ for Fe, $0.61\pm0.24\mu_B$ for Pt, and the orbital magnetic moment $-0.01\pm0.01\mu_B$ for Fe, $-0.10\pm0.10\mu_B$ for Pt. Calculated spin and orbital magnetic form factor are shown as solid lines in Figs. 1 and 2 respectively, where the theoretical curves reproduce the observed value. In conclusion we have succeeded in estimating the spin and orbital magnetic moment of Fe and Pt in Fe₃Pt by the XMD experiment.

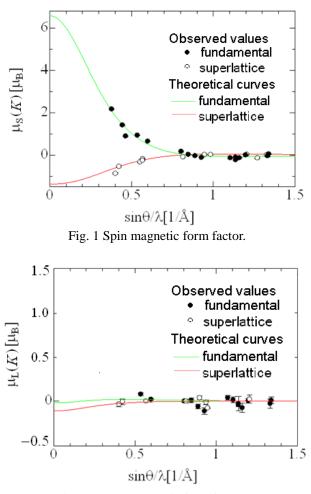


Fig. 2 Orbital magnetic form factor.

[1] International Tables for X-ray Crystallography Vol. IV (1974).

[2] K. Kobayashi, T. Nagao and M. Ito, Acta Cryst. A **67** (2011) 473.