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Estimation of order parameter in a binary alloy of Cu_3Au type structure by using white x-ray diffraction

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Introduction

A binary alloy of Cu_3Au structure shows order-disorder phase transition. Pd_3Co and Fe_3Pt belong to such crystal structure group. Hereafter we denote this type of alloys as A_3B. In the order phase of A_3B A atoms are located at the face center position of the cubic unite cell, while B atoms are located at the corner of the unit cell.

Structure factor of A_3B is expressed as follows. In the order phase, $F(hkl)=3f_A+f_B$ when h,k,l are all even or all odd, and, $F(hkl)=s(f_B-f_A)$ when h,k,l are mixture of even and odd number. In the disorder phase, $F(hkl)=3f_A+f_B$ when h,k,l are all even or all odd, and, $F(hkl)=0$ when h,k,l are mixture of even and odd number. Here, f_A, f_B are the atomic scattering factor of the A and B atom, respectively, and s is the order parameter that represents the degree of structural order ($0<s<1$). The state of $s=1$ denotes the perfectly ordered structure, and the state of $s=0$ denotes the completely disordered structure. Real crystal has an s value between them ($0<s<1$).

The present authors' group has been performing the X-ray magnetic diffraction (XMD) experiment of Cu_3Au type alloys. In the XMD data analysis of these alloy, exact value of the order parameter s has to be known. In this report we propose a method of estimating the order parameter s by white X-ray diffraction.

Experiments

Though Pd_3Co has been the main target of the XMD measurement on the beamline 3C, the present sample crystal alloy was revealed to be in the disorder state. So we utilize the XMD data of Fe_3Pt, which is another Cu_3Au type alloy in the order state, taken for $h00$ series of reciprocal lattice points on this beamline previously.[1)]

Results and discussion

The observed diffraction intensities $I_{obs}(E_{h00})$ for $h00$ (h =2,3,5,6) are plotted in Fig. 1 as solid squares, where E_{h00} is the X-ray energy. $I_{obs}(E_{400})$ is omitted because of severe disturbance from fluorescent Pt L X-rays to the diffraction peak. In Fig. 1 the ordinate is normalized by $I_{obs}(E_{600})$ where E_{600}=14.1keV. Then, we calculated the diffraction intensity $I_{cal}(E_{h00}) = I_0(E_{h00})|F(h00)|^2$ (h=2,3,5,6) for the perfectly ordered structure, where $I_0(E_{h00})$ is the X-ray intensity incident on the sample crystal. Here we estimated $I_0(E_{h00})$ by using the SPECTRA[2)] and by taking into account the absorption of X-rays by the Be windows and air in the beamline. The estimated $I_{cal}(E_{h00})$s' (h=2,3,5,6) are plotted in Fig. 1 as open circles. $I_{cal}(E_{h00})$s' are also normalized by $I_{cal}(E_{400})$.

By the above normalization, the relation $I_{cal}(E_{h00}) = I_{obs}(E_{h00})$ should hold for h=2 as well as for h=6. Slight disagreement of $I_{obs}(E_{200})$ from $I_{cal}(E_{200})$ could be due to slightly inadequate estimation of $I_0(E_{h00})$. In Fig. 1 for h = 3 and 5, $I_{obs}(E_{h00})$ is represented by $I_0(E_{h00})s^2|f_{Pt}-f_{Fe}|^2$, whereas $I_{cal}(E_{h00}) = I_0(E_{h00})|f_{Pt}-f_{Fe}|^2$. So for h = 3 and 5 the ratio $I_{obs}(E_{h00}) / I_{cal}(E_{h00})$ gives the s^2 values. From Fig. 1 we obtained s values for h = 3 and 5 as follows.

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$$s(300) = \sqrt{0.72/1.26} = 0.76,$$
$$s(500) = \sqrt{0.20/0.49} = 0.64.$$

Thus we have obtained the order parameter s≈0.7. Slight discrepancy between s(300) and s(500) might be due to also slightly inadequate estimation of $I_0(E_{h00})$.

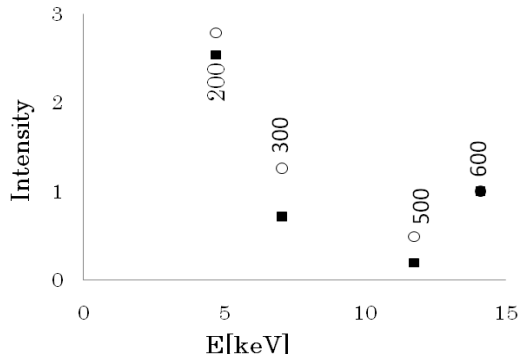

Fig. 1 Observed (■) and calculated (○)diffraction intensity of Fe_3Pt for reciprocal points of $h00$ (h=2,3,5,6).

References

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