

The effective charge on the Si atom in $\text{Fe}_x\text{Co}_{1-x}\text{Si}$ pseudobinary alloy

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Introduction

The pseudobinary alloys $\text{Fe}_x\text{Co}_{1-x}\text{Si}$ exhibit weak itinerant ferromagnetism at low temperature and have attracted much attention of many researchers in connection with verification of the spin fluctuation theory and with the characteristics of Kondo insulator. In these concerns, the main interest was concentrated on the host magnetic elements. Recently, we have performed soft X-ray fluorescence study at the Si *L*-edge [1] and have revealed the hybridization effect between Si and Fe or Co. The results are summarized as follow: with increasing 3*d* electron numbers by substituting Fe with Co, hybridization between Si 3*p* and transition-metal 3*d* orbitals is strongly enhanced. Considering the crystal structure of this alloy, B20 (a distorted rocksalt structure), the limbs of 3*d* orbitals should be elongated to the corners of a Si octahedron, e.g., *t*_{2g} orbitals hybridized with Si 3*p* ones. From the result of band-calculation [2], Si 3*p* states locate at binding energy (*E*_B) of ~4eV, whereas the crystal-field-split 3*d* states locate at *E*_B = ~1eV and ~3.5eV. Therefore, *t*_{2g} orbitals are more stable than *e*_g ones. In order to achieve this energy diagram, the effective charge on the Si atom should be positive.

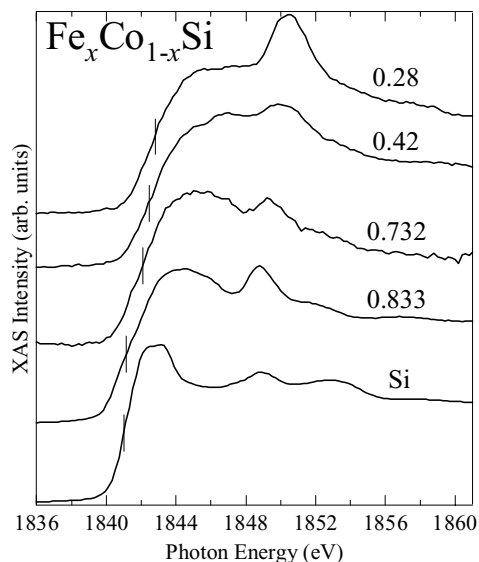
In this report, we present the X-ray absorption spectra of $\text{Fe}_x\text{Co}_{1-x}\text{Si}$ at the Si *K* edge and discuss about the hybridization effect based on a chemical shift of the edge.

Experimental

X-ray absorption spectra were taken at BL-11B with total electron yield method. The experiments were carried out under room temperature and high vacuum of the order of the order of 10⁻⁵ Torr.

Results and Discussion

Figure 1 shows the absorption spectra of $\text{Fe}_x\text{Co}_{1-x}\text{Si}$ at Si *K* edge for *x*=0.28, 0.42, 0.732 and 0.833 together with the spectrum of Si for comparison. The vertical bars indicate inflection points at edges. The chemical shifts relative to Si versus nominal number of 3*d* electrons are plotted in Fig. 2. Quite similar correlation obtained from the Si *K*α fluorescence spectra is reported by Liu *et al* [3]. From their result, the effective charges on Si are increased with the chemical shift in Si *K*α lines, namely Si is positively charged when the chemical shift is positive. Then, our result directly indicates that the effective charges on the Si atom in $\text{Fe}_x\text{Co}_{1-x}\text{Si}$ is positive and that the positive charge increases with increasing nominal



number of 3*d* electrons. This result is also consistent with our simple consideration described above.

References

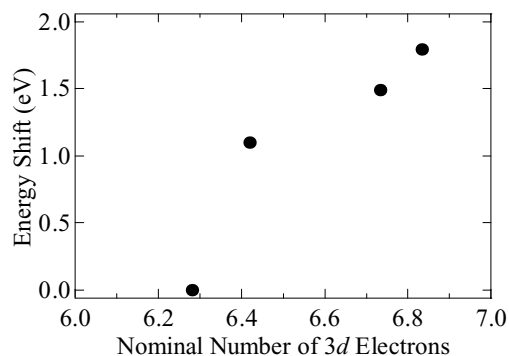


Fig. 2 Energy shift of Si *K*-edge versus the nominal number of 3*d* electrons.

Fig. 1 X-ray absorption spectra of $\text{Fe}_x\text{Co}_{1-x}\text{Si}$ at Si *K* edge for *x*=0.28, 0.42, 0.732 and 0.833 together with the spectrum of Si for comparison. The vertical bars indicate inflection points at edges..

- [1] N. Nakajima *et al.*, PF. Act. Rep. **22**, 102 (2005).
 [2] H. Yamada, private communication
 [3] Z. Liu *et al.*, Phys. Rev. **B69**, 035106 (2004); H. Ishii *et al.*, Phys. Rev. **B71**, 205202 (2005).

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