Asymmetry in the Mossbauer Spectra of Amorphous Fe_<100-x>B_x (14 x 21) Alloys

Asymmetry in the Mössbauer Spectra of Amorphous $Fe_{100-x}B_x$ ($14 \leq x \leq 21$) Alloys*

Hideya Onodera, Hisao Yamamoto and Hiroshi Watanabe

The Research Institute for Iron, Steel and Other Metals

(Received April 30, 1981)

Synopsis

The Mössbauer spectra of amorphous $Fe_{100-x}B_x$ ($14 \leq x \leq 21$) alloys which are slightly asymmetric are analyzed in terms of the distributions of hyperfine fields and isomer shifts. On the assumption that the correlation between hyperfine fields H and isomer shifts I.S. is described by I.S. = $c_0 + c_1 \cdot H$, where c_0 and c_1 are constants, the value of c_1 is dependent upon the concentration as same as c_0. While the change of c_0 is connected smoothly to the isomer shifts of crystalline α-Fe, Fe_2B and FeB, the value of c_1 which explains the asymmetry is sensitive to the amorphous structure.

I. Introduction

Numerous Mössbauer investigations have been reported on the ferromagnetic amorphous Fe-B alloys, because it is easy to prepare the samples and these alloys form one of the simplest binary system with one kind of magnetic atom like Fe-P and Fe-Si alloys. The Mössbauer spectra of these alloys show a slight asymmetry about the centroid. A few reports have dealt with this asymmetry in the calculation of the hyperfine field distributions, P(H). Vincze have indicated that a distribution of sizable effective EFG can be deduced from the spectrum of $Fe_{80}B_{20}$, but the recalculated full spectrum including this effect has not been reported.[1] In amorphous $(Fe_{0.2}Co_{0.8})_{80}P_{17}Al_3$, Chien and Chen have explained the asymmetry of spectrum with a distribution of isomer shifts, P(I.S.), and its correlation with a hyperfine field distribution.[2] Though it is desired to analyze actual spectra of amorphous alloys by using distributions and correlations of hyperfine fields, isomer shifts and EFG, it is practically too complicated.

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* The 1727th report of the Research Institute for Iron, Steel and Other Metals.

II. Procedure of Analysis

In the present paper, the Mössbauer spectra of the amorphous $Fe_{100-x}B_x$ ($14 \leq x \leq 21$) alloys at 20K are analyzed with a following procedure;

(1) P(H) is assumed to be a split Gaussian shape[3] which is described as,

$$P(H) \propto \begin{cases} \exp[- (H - H_0)^2 / 2\Delta_1^2], & H > H_0 \\ \exp[- (H - H_0)^2 / 2\Delta_2^2], & 0 \leq H \leq H_0, \end{cases}$$

and the correlation of isomer shifts with the hyperfine fields is

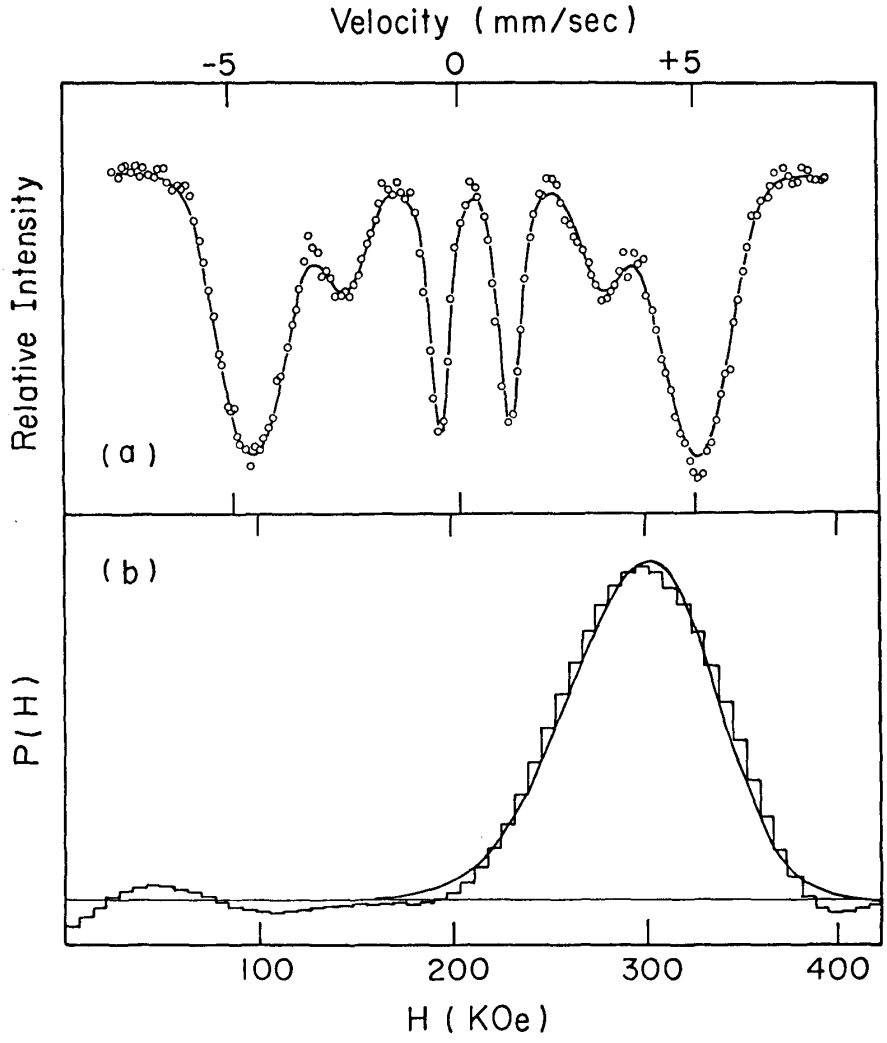

Fig. 1. (a) Observed and calculated spectrum, and (b) distributions of hyperfine fields of the amorphous $Fe_{83}B_{17}$ alloy. The solid curve is the distribution calculated as the split Gaussian, and the step function is obtained by the Hesse-Rübartsh method.

approximately described as I.S.(H) = $c_0 + c_1 \cdot H$. The values of H_0, Δ_1, Δ_2, Γ (a half width of elementaly Lorentzians), c_0 and c_1 are obtained with the least squares method.

(2) P(H) is recalculated with the Hesse-Rübartsch method[4] using the values of Γ, c_0 and c_1, and then the spectrum is calculated using this distribution function and the parameters.

III. Results and Discussion

As an example of the analysis, Fig. 1 shows the observed spectrum of $Fe_{83}B_{17}$ and the results of the calculation. The shape of P(H) obtained as the split Gaussian distribution is not much different from that calculated by the Hesse-Rübartsh method. It has been

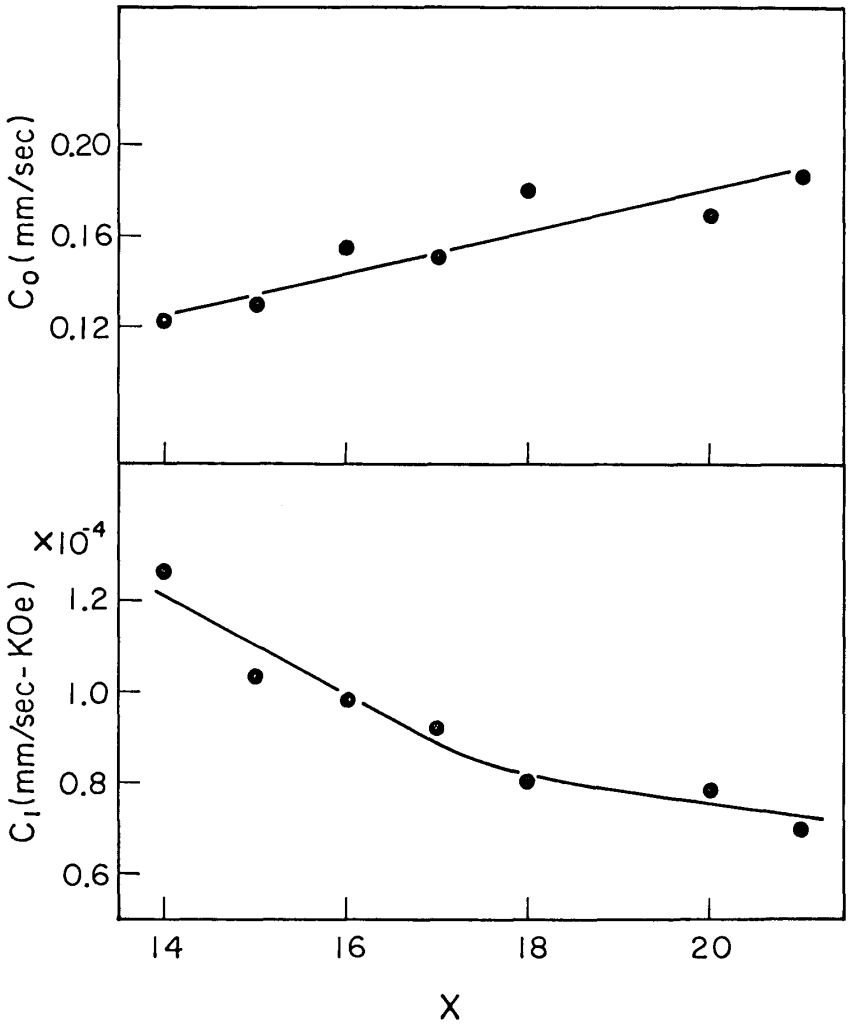

Fig. 2. Concentration dependences of C_o and C_1. The definitions of C_o and C_1 are in text.

reported [5] that the Gaussian approximation give a similar results to that obtained by the Fourier expansion method.[6] The values of Γ, c_0 and c_1 in $Fe_{83}B_{17}$ are 0.417mm/sec, 0.150mm/sec and 0.915×10^{4}mm/(sec·kOe), respectively. Fig. 2 shows the concentration dependences of c_0 and c_1. The parameter c_0 means the most probable isomer shift.[2] The fact that the values of c_1 are positive in the all compositions contradicts the case of $(Fe_{0.2}Co_{0.8})_{80}P_{17}Al_3$.[2] Inspecting the asymmetry of the spectra, however, it is considered that the values of c_1 are also positive in $Fe_{78}B_{12}Si_{10}$[7] and $Fe_{84}B_{16-x}C_x$.[8] It is highly likely that the alloys stabilized by a metalloid of B or C show the asymmetry described with the positive c_1 value and the alloys with P, Si or Al show the asymmetry with the negative one. In fact, the asymmetry of tbe spectra in $Fe_{80}Ni_{40}P_xB_{20-x}$ changes gradually with the increase of x,[9] and this phenomenon can be explained by the change of c_1 from positive value to negative one. Since the mean values of hyperfine fields and isomer shifts in the amorphous Fe-B system change monotonically with the concentration and agree with these of the crystalline α-Fe, Fe_2B and FeB by extrapolation and interpolation,[10] it appears that these mean values do not relate with the structure. It is supposed that the parameter of c_1, i.e., the asymmetry of the spectrum is sensitive to the amorphous structure . It is noted that the bend of the c_1 curve in Fig. 2 is observed at the concentration of $x\approx18$, and that the concentration dependence curve of density shows the bend at the value near to $x\approx18$.[11] The study of the dependence of c_1 on metalloid atoms is being prepared by the authors.

As shown in Fig. 1 (a), the inner four peaks have the asymmetry which is explained by the positive value of c_1, but the outer two peaks show the reverse asymmetry. All the alloys of $14\leq x\leq21$ in the present study show such asymmetries which have been also observed in $(Fe_xNi_{1-x})_{80}B_{20}$[9),12] and $Fe_{100-x}B_x$.[10] Since this complicated asymmetry is observed in intensities but not in peak positions, it is hard to consider that such asymmetry is caused simply by a residual EFG effect. A fruitful analysis need a definite correlation among hyperfine fields, isomer shifts and EFG's which distribute respectively.

Acknowledgement

We would like to thank Prof. T. Masumoto and the members of his laboratory for kind support and helpful advice in preparing the amorphous samples.

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