Mossbauer Spectra of Iron Sulfide Fe1-xS

V. 26 Mössbauer Spectra of Iron Sulfide $Fe_{1-x}S$

Igaki K., Sato M.* and Shinohara T.**
Department of Materials Science, Faculty of Engineering, Tohoku University
Graduate School of Tohoku University*
Research Institute for Iron, Steel and Other Metals, Tohoku University**

Iron sulfide $Fe_{1-x}S$ ($0 \leq x \leq 0.125$) takes various superstructures formed by the ordering of iron vacancies.[1] It has been reported on Mössbauer spectrum for the sample with x = 0.125 corresponding to stoichiometiric Fe_7S_8 that component spectra correspond to the iron sites having different configurations of surrounding iron vacancies.[2-3] But these correspondence has not been discussed yet on the sample with composition $x < 0.125$. The component spectra in Mössbauer spectra are investigated in this study.

The single crystal grown by the Bridgman method was used for the measurement. Samples were annealed at 900°C under the fixed sulfur pressures in order to control the sample composition, and were polished mechanically to about 100 μm thick. The spectra were measured at room temperature by the spectrometer with 2-3 mCi ^{57}Co in Rh matrix and fly back drive.

The obtained Mössbauer spectra could be divided into six portions corresponding to six lines by Zeeman splitting. Central portions were of nearly single peak independent of composition and the shape of outermost portions changed from three peaks to one broad peak with decreasing x from 0.125. This suggests that Mössbauer spectrum is composed of several components with different hyperfine fields and similar isomer shifts.

Each portion of spectrum was computerfitted as the superposition of Lorentzians with a common line width by the least squares iterative procedure in order to resolve finely the components. Figure 1 shows an example of analysis for the outermost portions for the sample with x = 0.095. Components were distinguished by letters as a, b, c, ... in turn from the outside of the left outer most portion. The spectrum for the sample with x = 0.125 was composed of three peaks a, f and i, another components appeared with decreasing x. The appearance of the outermost portion is considered to change to one broad peak for x close to 0.08, resulting from the increasing intensity of components c, d and e with decreasing x. Finally, nine components could be resolved, by comparing peak positions obtained on all specimens. The hyperfine parameters of nine components are given in Table 1. These hyperfine parameters were independent of the composition, and line width of a Lorentzian was nearly constant about 0.3 mm/sec. These components could be distinguished by main difference in the values of hyperfine fields.

The hyperfine field acting on a noticed certain iron nucleus is considered to reflect the different configuration of vacancies surrounding the iron atom because the magnetic couplings between iron ions are lost by the presence of

iron vacancies. Therefore it is thought possible to assign the obtained components to the different configurations of vacancies, and the information of vacancy arrangement could be obtained from the analysis of the composition dependence of the relative intensity of each component.

References

1) Nakazawa H. and Morimoto N., Mat. Res. Bull. 6 (1971) 345.
2) Levinson L. M. and Treves D., J. Phys. Chem. Solids 29 (1968) 2231.
3) Gosselin J. R., Townsend M. G., Tremblay R. J. and Webster A. H., Mat. Res. Bull. 10 (1975) 41.

Table 1. The hyperfine parameters of the obtained components

COMPONENT	H (kG)	Q.S. (mm/sec)	I.S. (mm/sec)
a	305 ± 5	0.05 ± 0.05	0.67 ± 0.05
b	297 ± 5	0 ± 0.05	0.75 ± 0.05
c	286 ± 5	0 ± 0.05	0.75 ± 0.05
d	275 ± 5	0 ± 0.05	0.70 ± 0.05
e	265 ± 5	0 ± 0.05	0.69 ± 0.05
f	255 ± 5	0.05 ± 0.05	0.65 ± 0.05
g	265 ± 5	0.46 ± 0.05	0.80 ± 0.05
h	237 ± 5	0.12 ± 0.05	0.72 ± 0.05
i	225 ± 5	0.15 ± 0.05	0.68 ± 0.05

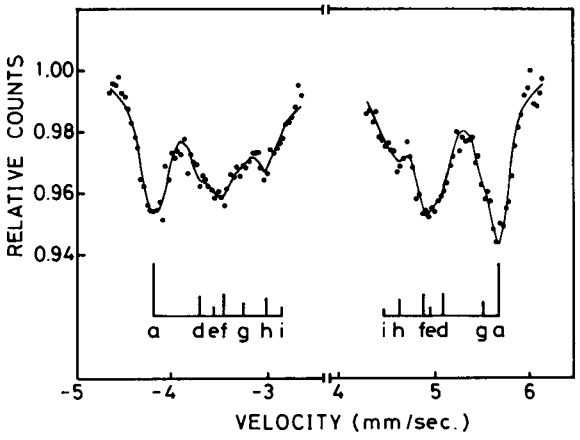

Fig. 1. The resolution of outermost portions in Mössbauer spectrum for the sample with x = 0.095 quenched from 900°C. The peak positions and relative intensities of components are indicated below the spectrum.