Journal of Magnetics 17(1), 6-8 (2012) http://dx.doi.org/10.4283/JMAG.2012.17.1.006

Mössbauer Study of the Dynamics in $BaFe_{12}O_{19}$ Single Crystals

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(Received 16 January 2012, Received in final form 30 January 2012, Accepted 30 January 2012)

Mössbauer spectra of hexagonal $BaFe_{12}O_{19}$ single crystals were studied at various temperatures (4-300 K). It was found that the spin states in Fe atoms were parallel to the γ-ray's direction into a single crystal along the c-axis. The location of the Fe ion in the 2b site is unusual in an oxide structure and has strong anisotropic lattice vibrations. Moreover, at room temperature, the zero absorption lines of the Fe ions at the 2b site were observed due to fast diffusion motion in a double well atomic potential. The two Fe ions of the single crystal mainly enter into the sites in the mirror plane of the trigonalbipyramidal structure.

Keywords : spin state, anisotropic lattice vibration, bipyramidal structure

1. Introduction

The barium ferrites belong to a large family of ferrimagnetic oxides with a hexagonal close-packed structure [1]. This M-type barium ferrite with a hexagonal molecular structure ($BaFe_{12}O_{19}$) is an important permanent magnetic material with interesting magnetic properties [2, 3] and thermal dynamics, such as large magnetocrystalline anisotropy [4], high Curie temperature, excellent chemical stability and corrosion resistivity [5].

Over the past 50 years, large research efforts into hexagonal M and W type ferrites have been made because of its relevance to certain technological applications and promising properties, such as for use in permanent magnets due to its high value of magnetization, in microwave devices for its microwave absorbing capability owing to its high permeability, and in magnetic recording media [1, 5-8].

Through the use of Mössbauer spectroscopy, information on magnetic structure can be obtained from these hexagonal barium ferrites [9].

The 2b site, which is one of the five crystallographically different lattice sites, is pentacoordinated within a trigonalbipyramid. The location of the Fe ion in the 2b site is unusual in this oxide structure and has strongly anisotropic lattice vibrations.

From experiments on $BaFe_{12}O_{19}$ single crystals the vibration mode of the Fe ion in 2b site has been found [10].

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2. Experiment

Single crystals of hexagonal ferrite $BaFe_{12}O_{19}$ were grown by the self flux method and crystals of up to 4 cm^2 in size were obtained. The uniqueness of the M type phase was verified by X-ray crystallographics.

The as-grown crystals have a platelet shape with the hexagonal c axis perpendicular to the face, the crystals were polished down to a thickness of 100 μm to act as Mössbauer absorbers. The sample was placed in a cryostat with the c axis parallel to the incoming γ-ray direction and Mössbauer spectra were recorded with a constant acceleration drive system in the temperature range 4.2-300 K.

3. Result and Discussion

The X-ray diffraction (XRD) pattern of a single crystalline Ba-ferrite sample is shown in Fig. 1. It can be observed from the figure that all the major planes (006), (008), (0010), (0014), (0016) and (0020) are present, which confirms the c-axis orientation of the crystal. Fig. 2 shows the Mössbauer spectra of a $BaFe_{12}O_{19}$ single crystal. The five different lattice sites give rise to a different subspectrums. The intensity of the lines in a given subspectrum is proportional to the number of iron ions at the corresponding lattice site and also to the Mössbauer recoil-free fraction. We found that the spin states in the Fe atoms were all parallel to the γ-ray's direction and the whole crystal bulk formed only one crystal with the same spin

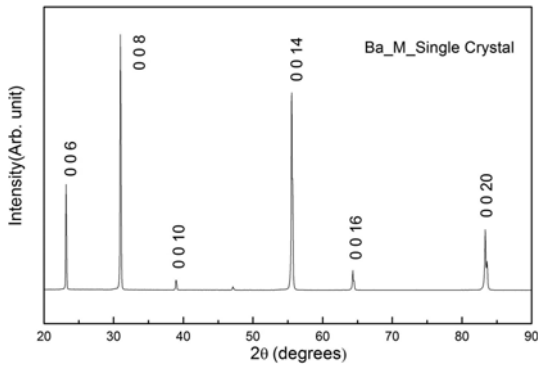

Fig. 1. X-ray diffraction pattern of a Ba-ferrite single crystal at room temperature.

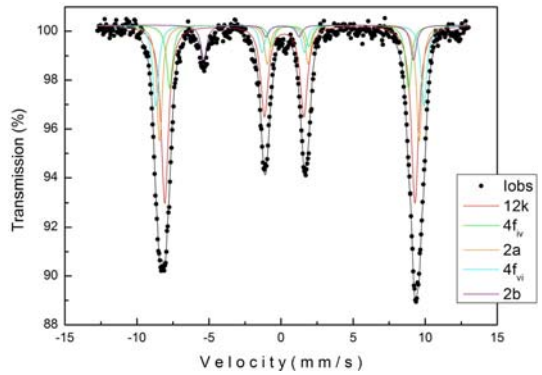

Fig. 2. (Color online) Mössbauer spectra of a $BaFe_{12}O_{19}$ single crystal and subspectra analysis at 4 K.

direction. However, in Fig. 3, the Mössbauer spectrum at 300 K has only four subspectra and the iron ions in the 2b sites show no absorption lines down to 180 K.

In Fig. 4 the Mössbauer spectra of the single crystal $BaFe_{12}O_{19}$ and its subspectra analysis as a function of temperature ranging from 4 K to 180 K are shown. The graph shows that at lower temperatures the 2b sites are observable. However, as the temperature increases the 2b

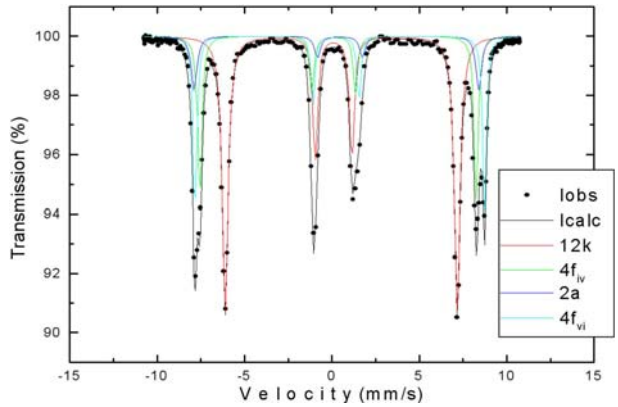

Fig. 3. (Color online) Mössbauer spectra of a $BaFe_{12}O_{19}$ single crystal and subspectra analysis at 300 K.

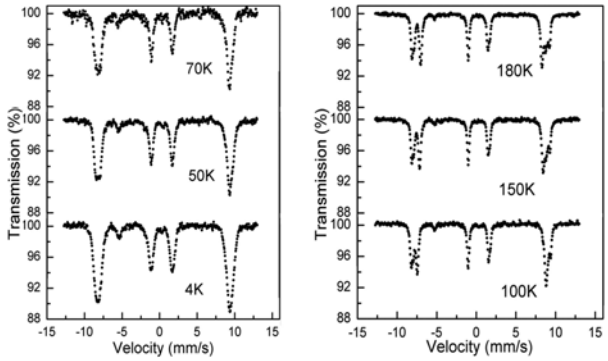

Fig. 4. Mössbauer spectra of a $BaFe_{12}O_{19}$ single crystal and subspectra analysis in the temperature range of 4-180 K

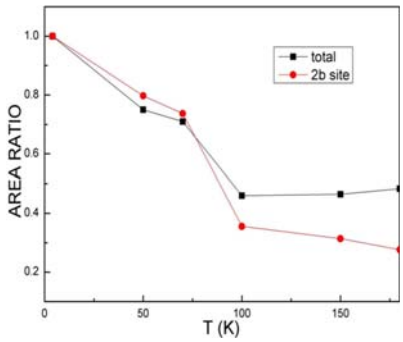

Fig. 5. (Color online) Plot of the Absorption Area of the Mössbauer Spectra at Various Temperatures

site absorption lines gradually diminish. Moreover, the plot of the ratio of the integrated 2b sites absorption area, shown in Fig. 5, shows the inverse relationship between temperature and absorption area. The absorption area computation is based on the 2b site area observed at 4 K. This may be attributed to the behavior of the iron ion's thermal motion is largely in the c-axis direction rather than at right angles to it.

This phenomenon can be related to the strong anisotropic Mössbauer recoil free fraction f, defined as $f = \exp(4\pi^2(-x_{av}^2/\lambda^2))$, where x_{av}^2 is the average of the square of the displacement of the Fe nucleus in the direction of the absorbed γ-rays and λ is its wavelength. The iron ions must have much larger thermal motion in the direction of the c-axis than at right angles to it [11]. The trigonalbipyramidal can be regarded as two tetrahedra sharing a face in the mirror plane. The iron ions in this 2b site exhibit very fast vibration along the trigonal axis.

4. Conclusion

In summary, we studied the dynamics of hexagonal $BaFe_{12}O_{19}$ single crystals from low temperature to room

temperature using Mössbauer spectra. The 2b sites that appeared at low temperature gradually scaled down as the temperature increased. This is due to the concurrent behavior of the Fe atoms in the direction of the γ-ray causing zero absorption that may be attributed to fast diffusion motion at room temperature. This occurrence can be further associated with strong anisotropic lattice vibration.

Acknowledgement

This paper was supported by Wonkwang University in 2010.

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