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DETERMINATION OF Fe AND Ni ORDERING IN TETRATAENITE FROM SAINT SEVERIN METEORITE USING SYNCHROTRON RADIATION*

by

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ABSTRACT

Measurement with synchrotron radiation shows that tetrataenite is metrically tetragonal. This lower symmetry is attained by ordering of Fe and Ni and their slight shifts from the averaged positions.

Key-words: Tetrataenite; Meteorite; Synchrotron; Radiation.

INTRODUCTION

Taenite is one of the Fe-Ni minerals which is commonly found in meteorites. The crystal structure of taenite is simply described as face-centered cubic structure, where all the atomic positions are occupied by Fe and Ni with equal probability. Its space group symmetry is Fm3m.

Tetrataenite is found only in the extremely slow-cooled meteorite (cooling rate of some degrees per million years for the temperature interval of 700 - 350°C). The structure of tetrataenite can be derived from taenite structure by ordering of Fe and Ni atoms and it is, therefore, described to be C-centered tetragonal and reduced to primitive tetragonal with:

$$\bar{a} = 1/2\bar{a}_c + 1/2\bar{b}_c$$

$$\bar{b}_p = 1/2\bar{a}_c - 1/2\bar{b}_c \quad \text{and}$$

$$\bar{c}_p = \bar{c}_c$$

(p = primitive lattice and c = C-centered lattice).

The space group symmetry has been described P4/mmm by Clarke and Scott (1980). The existence of the ordered tetragonal phase has been confirmed by optical observation and Mössbauer experiments. But the structure analysis of tetrataenite has not been carried out because of the difficulties to find good single crystal and to distinguish Fe and Ni with usual X-ray sources.

In this study, we report the results of the single crystal experiments on tetrataenite using sychrotron radiation, which is characterized by its strong intensity and the tunable wave length.

EXPERIMENTAL AND RESULTS

A single crystal of tetrataenite of 50μm in diameter could be separated from the Saint-Severin meteorite (type-LL6). The chemical composition was determined to be FeNi by means of the electron microprobe analysis. Lattice constants were determined by the four-circle diffractometer using Mo kα radiation are:

$$a = 3.577(2), \quad b - 3.576(3), \quad c = 3.569(2) \text{ A},$$

$$\alpha = \beta = \gamma = 90$$

(same orientation with FCC-lattice).

The crystal was then mounted on a four-circle diffractometer of vertical type on BL-10a in Photon Factory, Laboratory for High Energy Physics, Tsukuba. The diffraction data was collected with the ring current of 135-85 mA.

The X-ray of $\lambda = 1.746$ A was used to the experiment by Si(111) monochromator. The correction parameters for anomalous scattering are:

for Fe atom: $f' = -6.299$, $f'' = 0.469$ and

for Ni atom: $f' = -1.740$, $f'' = 0.638$

(Sasaki, 1984).

The large difference in f' and the small difference in f'' are very adequate to determine the site occupancies in the structure. A total of 56 reflections were collected with $10 < 2\theta < 100^{o}$.

The standard reflections measured at intervals of five reflections were used to the correction for decreasing intensity of the primary X-ray.

All the reflections which contradict with the extinction rule of the C-centered lattice symmetry were observed. Tetrataenite has P-lattice with lattice constants of a = b = 3.577 and c = 3.569 A. The structure determination was carried out using least squares program. On the first stage of the structure determination, the space group symmetry of P4mm was assumed, in which only occupational parameters, z - coordinates and temperature factors (anisotropic) of the atoms can be refined. R-factor was 12%. Then, the space group symmetry of Pm was assumed, where x-coordinates can additionally be refined. The final R-factor is 7%. The results of the refinements shows:

1 - Fe and Ni atoms are almost perfectly ordered and construct a layer-like structure.

2 - Fe and Ni atoms move of about 0.04 - 0.07 A from the positions of the disordered structure.

DISCUSSION

Tetrataenite was first found by its optical anisotropy, which indicates that it has a lower symmetry than cubic one. Then the lattice constants were measured and it was concluded that tetrataenite was tetragonal. According to the present results, tetrataenite is only metrically tetragonal and its structure has monoclinic symmetry. The lower symmetry was attained by the ordering of Fe and Ni and their slight shifts from the averaged positions.

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