AR-NE7/2011G652

Structure of $(Fe,Ni)_3S_2$ under pressure

Satoru Urakawa[1,*] Ryota Kamuro[1], Akio Suzuki[2], and Takumi Kikegawa[3]
[1]Department of Earth Science, Okayama University, Okayama 700-8530, Japan
[2]Department of Earth Science, Tohoku University, Sendai 980-8578, Japan
[3]Photon Factory, KEK, Tsukuba 305-0801, Japan

1 Introduction

The Earth and planetary cores are composed of iron-nickel alloy and some light elements. Sulfur is a primary candidate of lightening elements alloyed with iron-nickel. Therefore, phase relations and structure of the iron-nickel sulfides at high-pressures and temperatures are fundamental to study formation process and evolution of the planetary cores. Here we focus attention on iron-nickel sulfide $(Fe,Ni)_3S_2$. Fe_3S_2 is known to be stable above 14 GPa and affect the melting relations in the system Fe-FeS, but its crystal structure is still unknown [1]. On the other hand, Ni_3S_2 is stable even at 1 atm, which has trigonal symmetry with space group R32 (α-Ni_3S_2 heazlewoodite) [2]. This phase is known to transform into the high pressure orthorhombic structure with Cmcm symmetry at high pressures [3]. In this study we examine stability field of high-pressure phase of Ni_3S_2 and alloying effect of iron to its crystal structure.

2 Experiment

High pressure and temperature experiments were conducted at the pressures of 13 to 18 GPa and the temperatures up to 900 K using the MAX III system installed at PF-AR NE7. X-ray diffraction patterns were taken by an energy dispersive method using a Ge-SSD at Bragg angle of 6 degree. Pressure was evaluated by the unit cell volume of NaCl pressure marker. X-ray profiles were analyzed using the PD Indexer software package provided by Seto Y.

3 Results and Discussion

We observed the phase transformation from α-Ni_3S_2 to the orthorhombic structured-Ni_3S_2 between 300 K and 500 K around 15 GPa (Fig. 1). This is close to the phase boundary determined by the first-principle calculation [4]. It is, therefore, though to be reasonable that the high-pressure phase of Ni_3S_2 is stable above 15 GPa. The orthorhombic phase can be quenched to room temperature at high pressures, but it backs into α-Ni_3S_2 after decompression. We also observed $(Fe_{0.5}Ni_{0.5})_3S_2$ under pressure and found the orthorhombic structure stabilized above 700 K around 15 GPa (Fig. 2). Thus about 50 % Fe_3S_2 can dissolve into the high pressure Ni_3S_2 phase. This implies that Fe_3S_2 which is stable above 14 GPa may also take the orthorhombic structure with Cmcm symmetry.

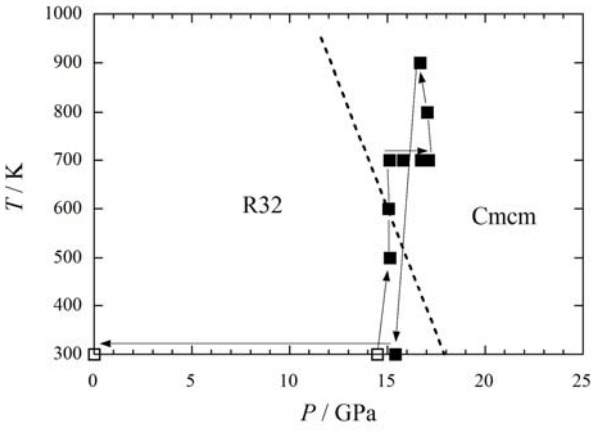

Fig. 1: The *P-T* path of in-situ observation of Ni_3S_2. Solid squares are the orthorhombic phase and open symbols are α-Ni_3S_2. Dashed line is a phase boundary evaluated by the first-principle calculation [4].

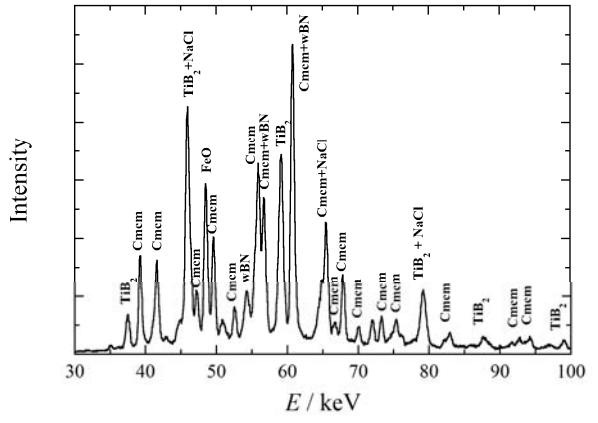

Fig. 2: Energy-dispersive X-ray diffraction profiles of $(Fe_{0.5}Ni_{0.5})_3S_2$.

References

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* urakawa@cc.okayama-u.ac.jp