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Structure and stability of Ni_3S under pressure

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Introduction

Planetary core are thought to consist of iron, nickel, and some light elements, such as sulfur. Iron-nickel sulfides are candidate constituents of planetary core and their physical properties are of important to investigate formation, evolution and present state of planetary core. We had found a new nickel sulfide phase with Ni_3S composition, which was observed as a liquidus phase in quenched samples from melts at 10 GPa [1]. We studied the structure and stability fields of Ni_3S using in-situ X-ray observation.

Experimental

High pressure and temperature experiments were conducted up to 10 GPa using the MAX80 system installed at PF-AR NE5C. X-ray diffraction patterns were taken by an energy dispersive method using a Ge-SSD. Pressure was evaluated by the unit cell volume of NaCl pressure marker.

Results and Discussion

Powder X-ray diffraction revealed that Ni_3S is isostructural with Fe_3S reported by Fei et al. [2], which has a Fe_3P-type structure with a tetragonal symmetry (space group I-4). Stability filed of Ni_3S was also determined by X-ray diffraction using a powder mixture of Ni and NiS with Ni_3S composition. Ni_3S forms above 5 GPa, and it breaks down into Ni and Ni_3S_2 below 5 GPa (Fig. 1). Ni_3S melts incongruently into Ni and liquid and its melting temperature gradually increases with pressure.

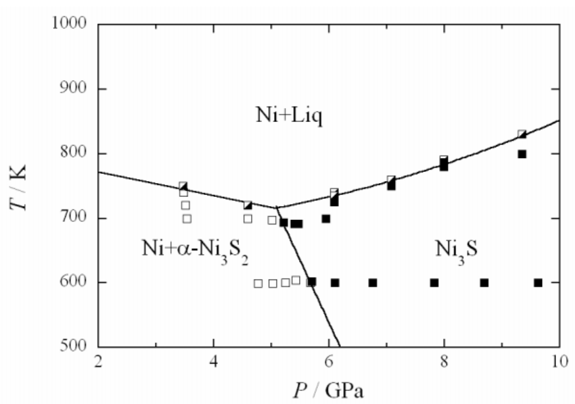

Fig. 1. Phase relations for Ni_3S.

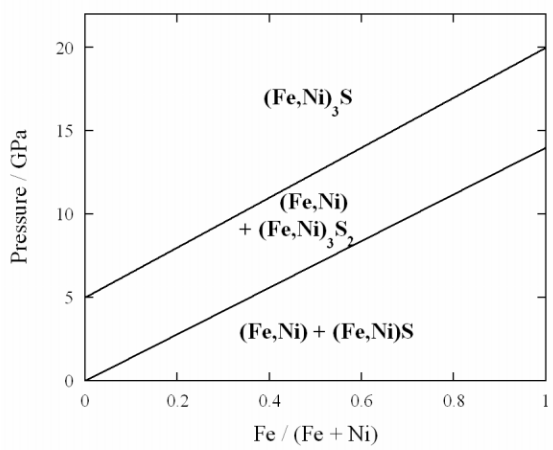

Fig. 2. Schematic phase diagram of $(Fe,Ni)_3S$ composition, indicating stability of $(Fe,Ni)_3S_2$ and $(Fe,Ni)_3S$.

Zhang and Fei [3] reported 50 % of Ni can substitute for Fe in Fe_3S at 20 GPa. Present results, therefore, suggest complete solid solution between Fe_3S and Ni_3S above 20 GPa. Fig. 2 shows the possible stability fields for Fe-Ni sulfides for $(Fe,Ni)_3S$ composition at high pressures. Intermediate sulfide compounds always appear at the lower pressure for the Ni-NiS system rather than the Fe-FeS system. Ni_3S_2 is stable still at the atmospheric pressure and Ni_3S forms above 5 GPa, whereas Fe_3S_2 and Fe_3S form at the higher pressure than 14 GPa and 20 GPa, respectively [2,4].

References

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