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Category: International Joint Research/ General Joint Research/ Joint Use of Facility/ Workshop

Name of the research project: Studies of the *P-V-T* equations of state of $(Fe,Ni)_2P$ and the *P-T* conditions of the "C22 to C23" phase transition

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Research report:

1. Research purpose

Iron-nickel phosphides, such as schreibersite [$(Fe,Ni)_3P$], barringerite [$(Fe,Ni)_2P$], allabogdanite [$(Fe,Ni)_2P$], and perryite [$(Fe,Ni)_8(Si,P)_3$], are often observed as common accessories in iron and stony-iron meteorites [1,2]. These phases have been suggested formed in the solar nebulae [3], but there is a strong argument that they might also have experienced later alterations, in the parent bodies or after delivery to the Earth [4]. Recently, $(Fe,Ni)_2(S,Si,P)$ has been suggested to be a possible constituent of the metallic planetary cores [5]. Knowledge of the high-pressure and high-temperature the Fe-Ni-P system are essential for constraints on physical and chemical properties of planetary cores and *P-T* histories of meteorites.

Despite the significance, the study of this issue is not adequate. Fe_2P has been observed to transform from barringerite (*P*-62*m*, C22) to allabogdanite (*Pnma*, C23) at 8 GPa and 1400 K, and the latter could be quenched to ambient conditions as a metastable phase [6]. However, the phase boundary of the C22 and C23 phases has not been well studied. The insufficient knowledge of the thermal equations of state (*P-V-T* EOS) and pressure-temperature (*P-T*) phase diagrams of the Fe_2P polymorphs limits fully characterization of the Fe-P system at high pressure and temperature. In this study, we plan to investigate the *P*-*V*-*T* EOS of allabogdanite Fe_2P and the *P*-*T* phase diagram of barringerite-allabogdanite $(Fe_{1-x}Ni_x)_2P$.

2. <u>Actually conducted research</u>

(1) *P*-*V*-*T* EOS of allabogdanite Fe_2P and *P*-*T* phase diagram of barringerite-allabogdanite Fe_2P

P-*V*-*T* equations of state of allabogdanite Fe_2P has been obtained up to 900 K and 11 GPa using the multi-anvil high-pressure experimental technique at beamline BL04B1 in the SPring-8 synchrotron facility. The phase boundary between C22 and C23 phases has been confirmed up to 17 GPa. Up to 5 GPa, the phase transition temperature from C22 to C23 was found at about 800 K, which is much lower than the previously reported 1400 K [6]. And after heating to 1200 K, the C23 phase will transform into the C22 phase. The narrow stability range of the C23 phase at low temperatures may suggest a special formation condition for nature allabogdanite in the meteorites and the C23 phase may exist in the cores of small-sized terrestrial planets with low internal pressure and temperature.

(2) *P*-*T* phase diagram of barringerite-allabogdanite $(Fe_{1-x}Ni_x)_2P$

Barringerite $(Fe_{1-x}Ni_x)_2P$ with various Ni contents, i.e., Fe_2P, $Fe_{1.9}Ni_{0.1}P$, $Fe_{1.5}Ni_{0.5}P$, and Ni_2P, were synthesized using a 14/8 cell assembly on the USSA-1000 multi-anvil apparatus at IPM. For studying the phase diagram, quenched experiments were performed at 8 GPa and 800, 900, 1000, 1100 K, kept for 12 h, using the USSA-1000 multi-anvil apparatus. Four barringerite samples, i.e., Fe_2P, $Fe_{1.9}Ni_{0.1}P$, $Fe_{1.5}Ni_{0.5}P$, and Ni_2P, were loaded in one 14/8 cell assembly. Recovered samples were characterized using micro-focused X-ray diffraction. Phases were confirmed as shown in Fig. 1. The allabogdanite $(Fe_{1-x}Ni_x)_2P$ existed in a narrow *T* range, and increasing Ni content played a negative role in its stability.

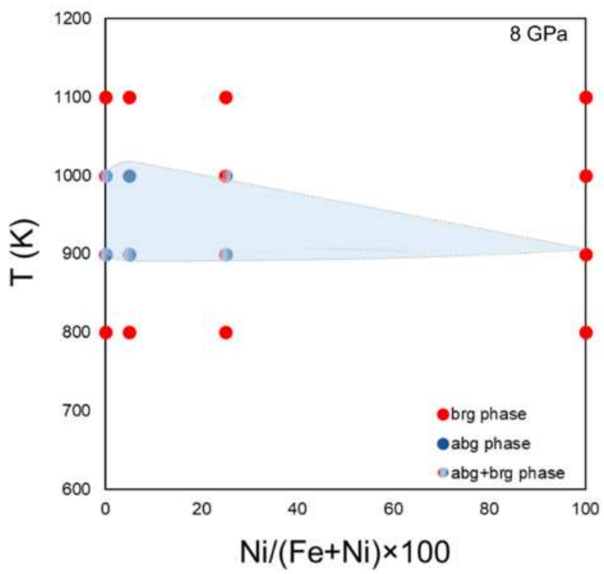

Figure 1. Phase diagram of barringerite-allabogdanite $(Fe_{1-x}Ni_x)_2P$ at 8 GPa, 800-1100 K.

References

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[3] Pataev and Wood, Lunar Planet. Sci. Conf., XXXI, 1608, (2000).

[4] Ivanova et al., Lunar Planet. Sci. Conf., XXXVI, 1054, (2005).

[5] Nakajima et al., Am Mineral, 105, 1752-1755, (2020).

[6] Dera et al., Geophys Res Lett 35:L1030, (2008).

3. Research outcomes

〇Zhang Y.*, He X., Yoshino T. (2023) Studies of the *P*-*V*-*T* equations of state of Fe_2P and the *P*-*T* conditions of the “C22 to C23” phase transition. IN: Japan Geoscience Union Meeting 2023: SIT18-P04. May 2023. Makuhari Messe, Chiba, Japan (Poster)

Zhang Y., He X., Yoshino T., Kagi H. *P*-*V*-*T* equations of state of allabogdanite Fe_2P and the “C22 to C23” phase transition of $(Fe_{1-x}Ni_x)_2P$. (Research paper in preparation)