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LETTER

New pressure-induced phase transition to Co_2Si-type Fe_2P

Yoichi Nakajima[1,*], Shunya Araki[1,2], Daisuke Kinoshita[1], Kei Hirose[3,4], Shigehiko Tateno[3], Saori I. Kawaguchi[5], and Naohisa Hirao[5]

[1]Department of Physics, Kumamoto University, 2-39-1 Kurokami, Chuo-ku, Kumamoto-shi, Kumamoto 860-8555, Japan
[2]Department of Physics, Faculty of Science, Kyushu University, 744 Motooka, Nishi-ku, Fukuoka-shi, Fukuoka 819-0395, Japan
[3]Earth-Life Science Institute, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku, Tokyo 152-8550, Japan
[4]Department of Earth and Planetary Science, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan
[5]Japan Synchrotron Radiation Research Institute, SPring-8, 1-1-1 Kouto, Sayo, Hyogo 679-5198, Japan

Abstract

We found a new phase transition in Fe_2P from Co_2P-type (C23) to Co_2Si-type (C37) structure above 42 ± 2 GPa based on in situ X-ray diffraction experiments. While these two structures have identical crystallographic symmetry, the orthorhombic unit cell is shortened in *a*-axis but elongated in *c*-axis, the coordination number of phosphorous increases from nine to 10, and the volume reduces by 2% across the phase transition. The new C37-type Fe_2P phase has been found to be stable, at least to 83 GPa at high temperature. The Birch-Murnaghan equation of state for C37 Fe_2P was also obtained from pressure-volume data, suggesting that phosphorous contributes to 17% of the observed density deficit of the Earth's outer core when it includes the maximum 1.8 wt% P as observed in iron meteorites. In addition, since both Fe_2S and Ni_2Si are also known to have the C37 structure under high pressure, $(Fe,Ni)_2(S,Si,P)$ could have wide solid solution and constitute planetary iron cores, although it is not dense enough to be a main constituent of the Earth's inner core.

Keywords: Iron phosphides, Fe_2P, high pressure, core, light element