PF-AR NE1A/2012G675

New high-pressure polymorph of In_2S_3 with defect Th_3P_4-type structure

Xiaojing Lai[1], Feng Zhu[1], Rong Huang[1], Xiang Wu[1], Shan Qin[1,*], Takumi Kikegawa[2]
[1]Peking University, Beijing 100871 China
[2]Photon Factory, Tsukuba 305-0801, Japan

1 Introduction

Indium sulfide (In_2S_3) is a sesquisulfide of group IIIA elements in the Periodic Table. It belongs to chalcogenide semiconductor, which has a potential application in photovoltaic devices area [1-3]. At ambient conditions, In_2S_3 crystallizes in a deficient spinel structure (β-phase, $I4_1/amd$, Z = 16). A high-pressure modification of In_2S_3 with corundum structure (ε-phase, $R\bar{3}c$, Z=6) has been identified by Range and Zabel [4]. No other study was done to the high-pressure behaviour of In_2S_3. Since A_2B_3-type sulfides provide implications about the structural behavior of the Earth's mantle minerals, especially the $(Mg,Fe)SiO_3$ perovskite (Pv), we here report the results of the high-pressure synchrotron XRD study of In_2S_3.

2 Experiment

The In_2S_3 sample with a purity of 99.99 % was purchased from Alfa Aesar. The sample was characterized by XRD at ambient conditions, which clearly showed that it was β-phase ($I4_1/amd$ and Z = 16) without any impurity.

Two runs of *in situ* high pressure synchrotron X-ray powder diffraction experiments using diamond anvil cells (DAC) were conducted at beamline PF-AR NE1 of KEK. High-temperature annealing was employed at certain pressure in these two runs by a portable laser heating system to overcome the potential kinetic effects on the phase transition and relax the stress gradient in the DACs.

3 Results and Discussion

The XRD patterns after laser-annealing in both runs show a new phase different from the β-phase. By indexing the peaks, we found this phase belongs to a defect Th_3P_4-type structure ($I\bar{4}3d$ and Z=5.333). Fig. 1 shows the Rietveld refinement of this phase at 35.6 GPa and 69.4 GPa, respectively. The refinement results were shown in Table 1.

Table 2. Crystallographic data for defect Th_3P_4-type In_2S_3 ($In_{2.667}\square_{0.333}S_4$, $I\bar{4}3d$ and Z = 4).

	35.6 GPa	69.4 GPa
a (Å)	7.557(1)	7.2423(5)
V (Å^3)	431.6(2)	379.87(8)
In1(12a)[a]	(0.375,0,0.25)	(0.375,0,0.25)
S1(16c)[a]	(0.083,0.083,0.083)	(0.083,0.083,0.083)
U_{iso}(In)	0.023	0.002
U_{iso}(S)	0.080	0.016
wR_p %	5.62	2.01
R_p %	3.31	1.56

[a] Atomic positions not refined.

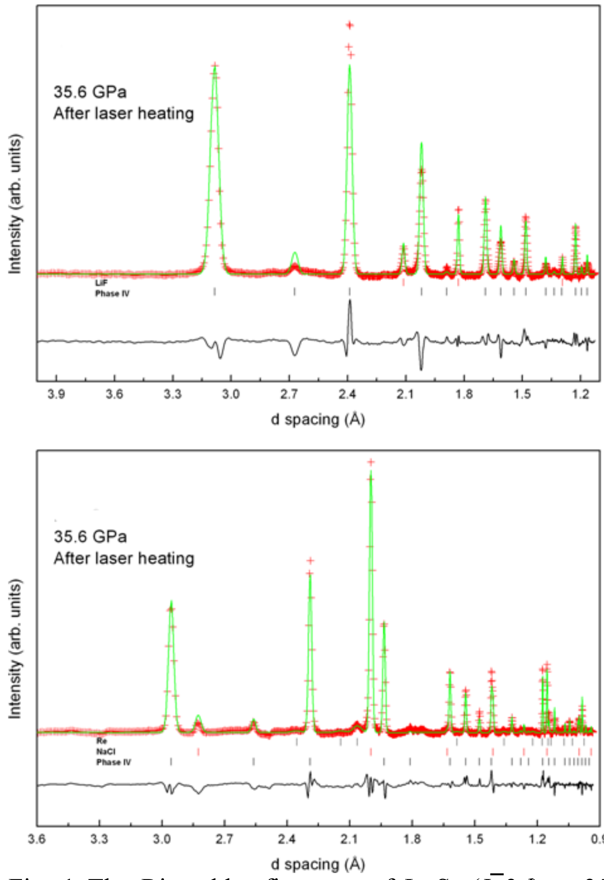

Fig. 1 The Rietveld refinement of In_2S_3 ($I\bar{4}3d$) at 35.6 Gpa and 69.4 GPa after laser heating. Measured (red crosses) and calculated (green continuous line) intensities, positions of the reflections (red, black, blue short bars) and difference curve (black line) between observed and calculated spectra are shown.

Acknowledgement

This work was supported by Natural Science Foundation of China (grant no. 41072027, 11079009 and U1232204). The authors would like to thank PF staffs for their help in the experiments.

References

[1] P.P. N. Revathi and K.T. Ramakishna Reddy, Energy Procedia **2** 195-198 (2010).
[2] A.M.V. Niyum *et al.*, Physica B **35**0 383-385 (2004).
[3] J.R. L. Aldon *et al.*, Phys. Rev. B **58** 11303-11312 (1998).
[4] K. Range and M. Zabel, Z. Naturforsch. B **33** 463-464 (1978).

* sqin@pku.edu.cn