

Pressure-induced structural change of unfilled skutterudite compound IrSb₃

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Introduction

Filled skutterudite compounds attracted many researchers' interest as strongly correlated electron systems. The skutterudite family includes binary, unfilled skutterudite compounds. The compounds crystallize in a body centered cubic structure of space group $Im\bar{3}$ and the binary compounds have a general formula TX_3 ($T=Co, Rh$ and Ir , $X=P, As$ and Sb , site $24g$) or $\square T_4X_{12}$ where the symbol \square represents a vacancy (site $2a$). While earlier studies indicate that the binary skutterudites are quite stable under high pressure, the structural change of $CoSb_3$ under high pressure has been reported, recently [1]. Our experiments have verified the phenomenon [2]. On the other hand, it has been reported that isostructural family $IrSb_3$ shows structural stability stable in the structure up to 42 GPa [3]. Therefore, we have studied the powder x-ray diffraction of $IrSb_3$ using synchrotron radiation, under high pressure in order to confirm structural stability of their compounds.

Experimental

High quality polycrystalline sample of $IrSb_3$ were prepared at 2GPa and 550°C, using a cubic-anvil high-pressure apparatus. The high-pressure diffraction experiments were performed at the beam line BL-18C. The powder x-ray diffraction pattern of $IrSb_3$ was measured with a diamond-anvil cell (DAC) and the imaging plate up to 40GPa at room temperature. Pressure in the DAC was determined from a pressure shift in the sharp R-line fluorescence spectrum of ruby. A 4:1 methanol-ethanol solution was used as pressure medium.

Result and discussion

Figure 1 shows x-ray diffraction patterns of $IrSb_3$ at several pressures. Vertical lines on this figure show peak positions at 1atm. No major change such as the appearance of any new peak was observed in the profiles of $IrSb_3$ obtained at pressures up to 40 GPa. This indicates that there is no change in crystal structure type within this pressure range. Although the sample was compressed normally up to 29 GPa, the intensity of 110 and 211 Bragg peaks was drastically suppressed at 40 GPa (Fig. 1(c)). Furthermore, the suppressed intensity of these peaks was maintained at the diffraction pattern after decreasing pressures (Fig. 1(d)).

Figure 2 shows the relative unit cell volume (V/V_0) of $IrSb_3$ versus pressure. V_0 is the volume at ambient pressure. Above 29 GPa, upon increasing pressure, the volume reduction with pressure becomes to be saturated and the volume decreases again in the range of over 40 GPa. Further, upon pressure release from 41 GPa, the cell

volume becomes greater than that observed at increasing pressure. This effect is irreversible, and the sample recovered at ambient pressure exhibits a volume about 2.3% greater than that of pristine $IrSb_3$. A similar behavior has been observed for $CoSb_3$ [1, 2]. The bends around 10 GPa are due to solidification of the 4:1 methanol-ethanol solution used as pressure medium.

This results suggests that the pressure-induced structural change is a common feature of unfilled skutterudite.

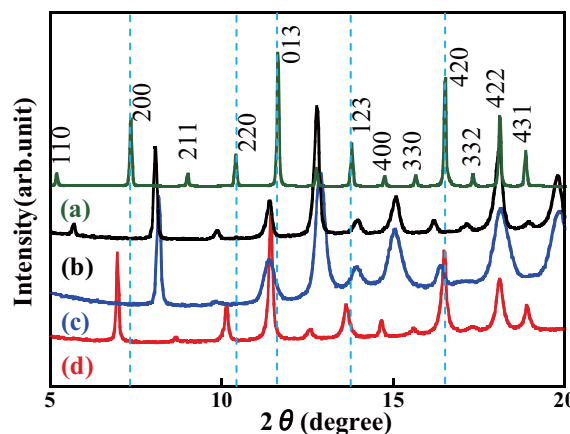


Fig.1. X-ray diffraction patterns of $CoSb_3$ at (a) 1 atm, (b) 29 GPa, (c) 40 GPa and (d) 0.1 atm (at decreasing pressure).

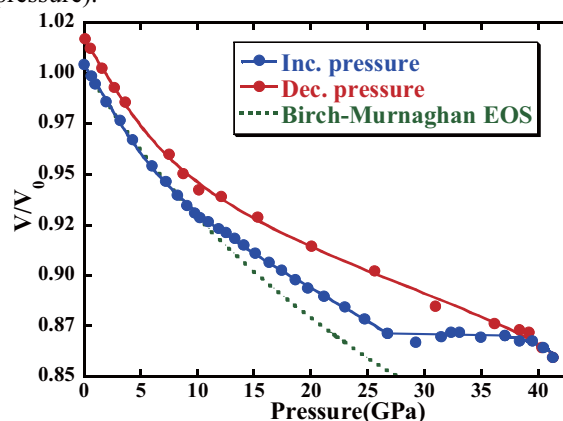


Fig.2. Pressure dependence of the relative unit cell volume for $CoSb_3$.

References

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