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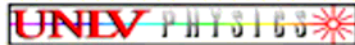
Study of Thermoelectric Materials at High Pressure

It is of extreme importance to develop new potential energy sources to reduce dependence on fossil fuels. As a result of this, the study of thermoelectric materials, capable of changing heat into electrical energy, has become a field of great interest regarding fundamental properties. To help better understand these materials, facilities for the measurement of relevant properties at high pressure have been developed, but lack the ability to characterize the materials at high temperature and pressure. Therefore, this project has the goal of developing a heater arrangement to be used in conjunction with the high pressure capabilities already developed to fully characterize these materials.

Structural studies of CrSi₂ at high pressures and temperatures

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High Pressure Collaborative Access Team



INTRODUCTION

Transition metal dichalcogenides have found important technological applications in silicon based microelectronics due to their high temperature stability and thermoelectric properties [1]. CrSi₂ is an indirect band gap semiconductor with an energy gap of 0.35 eV and could find potential applications in the Schottky barrier solar cell applications [2,3]. Because of its high melting point of the hexagonal CrSi₂ type structure, oxidation resistance and widebanding to stretching and deformation it is regarded as one of the promising structural materials for aerospace and energy applications [4]. It is also a potential thermoelectric material that can be utilized for generating electric power at high temperatures [5]. The figure of merit of CrSi₂, $2.8 \times 10^{-4} \text{ deg}^{-1}$ is comparable to the most superior chalcogenide thermoelectric materials [6]. As the high temperature and the thermoelectric applications depend mainly on the structural stability at the operating conditions, we intend to study the structural behavior of this material at high pressure and temperature. We have performed in-situ single domain powder x-ray diffraction up to 40 GPa and also investigated the structure by varying temperature.

EXPERIMENTAL DETAILS

High pressure x-ray diffraction experiments at room temperature were performed at the high resolution diffraction beam line ID-B, Sector 16 of Advanced Photon Source (Fig. 2a). Highly pure CrSi₂ (99.9%) polycrystalline sample was obtained from Sigma-Aldrich. The powder was well ground in an agate mortar and pelleted. A small piece cut from the dense pellet was loaded into a 130 μm hole of a stainless steel gasket of a Mao-Bell type diamond anvil cell with a ruby ball and poly-dimethyl siloxane pressure medium as shown in Fig. 2b.

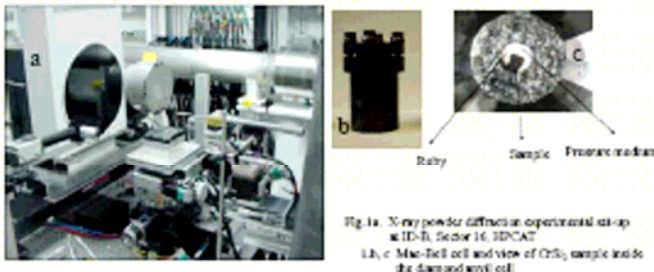


Fig. 1. X-ray powder diffraction experimental set-up at ID-B, Sector 16, 3DPCAT. (b), c Mao-Bell cell and view of CrSi₂ sample inside the diamond anvil cell.

Diffraction patterns were collected up to 40 GPa on a MAR 345 imaging plate using an incident x-ray wavelength of 0.42247 Å. The typical exposure time was 10 sec for each pressure. The sample to detector distance was calibrated using CeO₂ standard. The pressure inside the diamond anvil cell was determined using ruby fluorescence method [7]. The images were then integrated using FITD package and analyzed using JADE powder diffraction analysis software. Temperature dependent x-ray diffraction spectra were collected at ambient pressure from 273 K to 593 K for CrSi₂ powder at Chonmaeok-department, UNLV using a PANalytical diffraction system operating with a CuK α target.

RESULTS AND DISCUSSION

CrSi₂ crystallizes in the hexagonal P6322 structure (space group no.180) as reported elsewhere [8]. The Cr atoms occupy the 3d positions and the Si atoms are located at 6j positions (see the inset in Fig. 3). The cell parameters obtained at ambient conditions $a = 4.4330(1)$ Å and $c = 6.387(9)$ Å agree well with the literature [15].

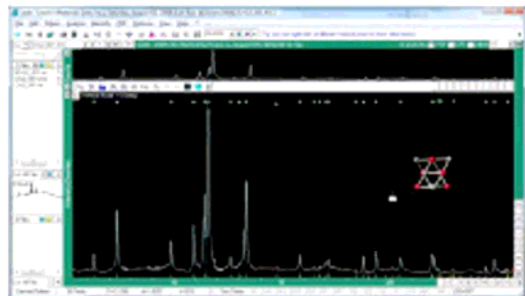


Figure 2. Image of the JADE window showing the diffraction pattern collected at 0.3 GPa fitted to the hexagonal cell. The hexagonal unit cell simulated using JADE & Siusis software is shown in the inset.

In Fig. 3 a, we have shown the evolution of diffraction patterns collected up to 40 GPa. The spectra were observed to be similar up to the highest pressure achieved in the experiment which showed no pressure induced structural phase transition. The unit cell volume as a function of pressure is shown in Fig. 3b. The P-V data were fitted to a second order Birch-Murnaghan equation shown below [10]

$$P = 3/2 B_0 [(V/V_0)^{2/3} - (V/V_0)^{1/3}] [1 + B_0' (V/V_0)^{1/3} - 1]$$

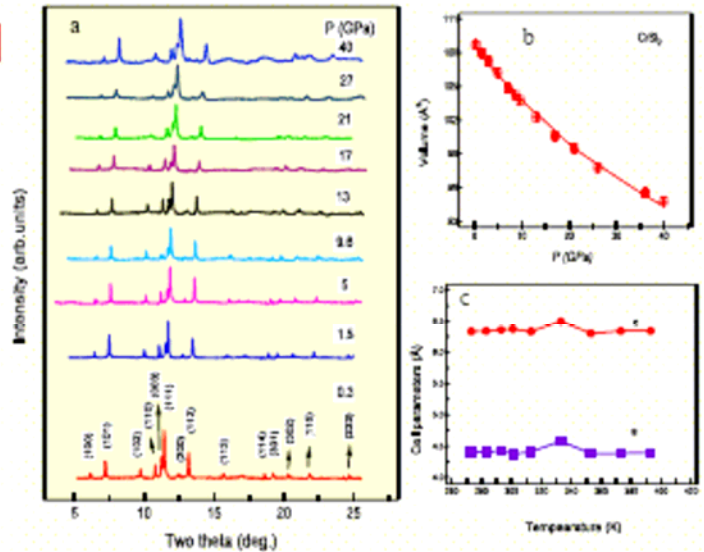


Figure 3a. Representative diffraction patterns collected at high pressure for CrSi₂.
 2b. Pressure-volume data (symbols). The dashed line shows the fit to Birch-Murnaghan equation (see text).
 3c. Variation of cell parameters as a function of temperature.

We have obtained a bulk modulus value of 208 (5) GPa with a first pressure derivative k' . We have compared the bulk modulus value with similar diatomic material FeSi₂ ($B_0 = 243$ GPa) which was studied by Mori *et al.*, and Ti-Si alloys [11,12]. We found that the bulk modulus value of CrSi₂ lies in between those two compounds. Nishitani *et al.* studied the chemical bonding of 3d transition metal dichalcogenides theoretically and reported that the strength of the transition metal (TM)-silicon (Si) bonding increases while Si-Si bonding decreases, when 3d TM goes from left to right on the periodic table [13]. As the Ti-Si bonding contributes mainly to the overall bonding in this system, we could conclude that the increase in the Ti-Si bonding increases the bulk modulus value when going from Ti to Fe.

We have analyzed the temperature dependent x-ray diffraction spectra collected by using the software program called Crystalball [14]. The cell parameters obtained were plotted as a function of temperature and shown in Fig. 3 c. From the diffraction results we have noticed no temperature induced structural phase transition either by cooling below ambient or raising the temperature up to 593 K. CrSi₂ was studied by Ma *et al.*, up to 7000C and they have shown that the hexagonal structure is stable in air [15]. Our results are consistent with the experimental observation.

CONCLUSIONS

We have performed high pressure and high temperature structural studies on CrSi₂. The high pressure experimental results indicate that the hexagonal structure of CrSi₂ is stable up to 40 GPa. The structure was further found to be stable as varying temperature from 273 K to 593 K. The bulk modulus obtained for CrSi₂ is comparable with other transition metal dichalcogenides. The high temperature x-ray diffraction results are consistent with the structural studies reported earlier. Our experiments confirm that, due to its structural stability, CrSi₂ could be used as an excellent high temperature material under extreme P-T conditions.

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