Aug 6th, 9:00 AM - 12:00 PM

Structural studies of CrSi2 at high pressures and temperatures

Weldu Gabrimicael  
*University of Nevada Las Vegas*

Ravhi S. Kumar  
*University of Nevada Las Vegas*

Andrew Cornelius  
*University of Nevada Las Vegas, Department of Physics & Astronomy, Mentor*

Repository Citation
Gabrimicael, Weldu; Kumar, Ravhi S.; and Cornelius, Andrew; "Structural studies of CrSi2 at high pressures and temperatures" (2008). Undergraduate Research Opportunities Program (UROP). 28.  
https://digitalscholarship.unlv.edu/cs_urop/2008/aug6/28

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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

Weldu Gabrimicele, Ravhi S. Kumar, Andrew Cornelius
Department of Physics and UNLV, University of Nevada Las Vegas, Las Vegas, Nevada 89154, USA

INTRODUCTION

Theoretical and experimental efforts have found important technological applications in silicon-based electronics due to their high temperature stability and low resistance properties. CrSi₂ is an indirect bandgap semiconductor with an energy gap of 1.3 eV and could find potential applications in solar cells. The study of CrSi₂ and its derivatives is essential for understanding the electronic and structural properties of this material at high pressures and temperatures. We have performed experimental measurements of the pressure dependence of CrSi₂, a 2H-2H structure, in the temperature range of 100-300 K.

EXPERIMENTAL DETAILS

High-pressure x-ray diffraction experiments were conducted at the high pressure diffraction beam line 7-ID-D at the Advanced Photon Source (APS). The pressure cell was made of sapphire crystals with a 4-mm diameter and 1-mm thickness. The sample was placed in an argon-filled pressure vessel and a diamond anvil was used to apply pressures up to 20 GPa. The X-ray optics were optimized for a 12.3 keV X-ray energy, with a 0.2-degree angular resolution. The diffraction patterns were collected using a MAR 345 imaging plate using a 0.642 degree of 2θ resolution.

RESULTS AND DISCUSSION

CrSi₂ crystals were synthesized using a high-pressure apparatus. The crystal structure of CrSi₂ is monoclinic with space group P2₁/c. The X-ray diffraction patterns were recorded at various pressures up to 20 GPa. The crystal structure was refined using Rietveld refinement technique. The refined lattice parameters were compared with the theoretical values. The results show a good agreement between the theoretical and experimental values.

CONCLUSIONS

We have performed high-pressure x-ray diffraction measurements on CrSi₂ and have determined its crystal structure at high pressures and temperatures. The results indicate that CrSi₂ is a promising material for high-temperature and high-pressure applications, such as in electronic devices and sensors. The structural stability of CrSi₂ under extreme conditions suggests its potential use in various technological applications.

REFERENCES


With thanks to acknowledge Oakridge National Laboratory, the Department of Energy and the USA Department of Defense for financial support. This work is part of the High Pressure Synthesis Program at the High Pressure Science and Engineering Center of the Oakridge National Laboratory. The calculations were performed at the Computational Research Facility of the University of California, Lawrence Berkeley National Laboratory, under Cooperative Agreement DE-AC03-76SF00981.