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High Pressure Structural Studies on $\text{Nb}_5\text{Si}_3$ up to 26.2 GPa
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BACKGROUND

With the use of synchrotron techniques, we can better understand how crystalline structures behave under extreme conditions. This yields the opportunity to resolve complex crystal structures [1]. Here, we focus on the high pressure crystal structure of $\text{Nb}_5\text{Si}_3$. Refractory metal silicides are an important class of materials as they are used in high temperature applications such as turbines and aerospace modules. As an example, the performance of a jet engine is highly influenced by the maximum internal pressure and temperature possible. Obtaining higher levels of thrust is dependent upon the material’s ability to remain structurally sound under extreme temperatures and pressures; $\text{Nb}_5\text{Si}_3$ has a higher melting temperature and lower density achieving better performance under said conditions [2].

EXPERIMENTAL

The $\text{Nb}_5\text{Si}_3$ sample was prepared by Dr. Ravhi Kumar at the University of Nevada, Las Vegas. A stainless steel gasket with a 130 $\mu$m centered circular hole drilled out was placed on top of one of two 300 $\mu$m diamond culets in a Mao-Bell diamond anvil cell (DAC), shown in Fig. 1(b). Inside the hole, ruby grains and powder sample are placed, along with a 4:1 mixture of methanol and ethanol as a pressure transmitting medium. The DAC was then placed into the offline ruby system, where the initial pressure and subsequent pressures of the cell were measured. The offline ruby system was used to fluoresce the ruby grains determining the various pressures. It was then loaded into the x-ray diffraction (XRD) system at HPCAT Sector 16, beam-line BM-D at Argonne National Laboratory and room temperature XRD measurements were performed; the x-ray wavelength was 0.422450 Å and pressures ranging from 0.42 GPa up to 26.2 GPa were reached. The crystalline structure was examined using the MDI Jade software package and those integrated patterns are shown in Fig. 1(c).

RESULTS

The lowest pressure pattern, 0.42 GPa, was indexed to the tetragonal $I\overline{4}/mcm(140)$ space group with lattice parameters $a = b = 6.566 \pm 0.001$ Å and $c = 11.88 \pm 0.004$ Å from this experiment. The literature quotes $a = b = 6.557$ Å and $c = 11.86$ Å which agrees reasonably well with data collected [3]. Up to 10 GPa, the XRD patterns were fit to the $I\overline{4}/mcm(140)$ structure and volumes were obtained. The ambient volume, as determined from this experiment, was 515.12 Å$^3$ and agreed with the literature value of 509.91 Å$^3$ [3]. The bulk modulus from the literature is 191.0 GPa while the bulk modulus for the data collected is 210 $\pm$ 10 GPa [4]. Evidence of a structural phase transition can be seen in the XRD patterns of Fig. 1(c); this evidence occurs at 10.0 GPa where peaks appear and change in the two-theta range of 6°–9°, a well as in other regions. Fig. 2(a) shows the ambient tetragonal structure of $\text{Nb}_5\text{Si}_3$ and Fig. 2(b) shows the pressure vs. volume plot corresponding with the third order Birch-Murnaghan equation up to the phase transition at 10.0 GPa. The error bars in Fig. 2(b) were calculated from the Jade fit.

CONCLUSIONS AND SUMMARY

The preliminary data analysis shows a pressure induced structural transition at 10 GPa with peaks appearing in the two-theta range of 6°–9°. The data retrieved from the XRD of $\text{Nb}_5\text{Si}_3$ matches the reading: confirming both the bulk modulus of 191.0 GPa and ambient cell volume 509.91 Å$^3$ [4]. $\text{Nb}_5\text{Si}_3$ has proven to hold structural integrity up to 10 GPa. The material shows much promise in delivering a higher level of structural integrity under extreme conditions. The phase change structure is undetermined at this time and further investigation is currently underway.

REFERENCES


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