PRESSURE-INDUCED PHASE TRANSITIONS OF SILICIDES

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Introduction

We have studied pressure effect on alkaline-earth-metal disilicides because their structures have characteristic Si configurations. In situ x-ray diffraction measurements of $BaSi_2$ showed that the structure changes from orthorhombic to cubic, then to trigonal with increasing pressure. [1, 2] The cubic and the trigonal structures are almost the same as those of $SrSi_2$ and $CaSi_2$ at ambient conditions, respectively. Thus, the structures that appear at high pressure are the same as those at ambient conditions of the other alkaline-earth-metal disilicides with a smaller atomic number metal. This structural sequence is different from those known in elements and the other AB_2-type compounds such as dioxides of 14 group elements. For better understanding of the structural sequence, pressure experiments are necessary for the other alkaline-earth-metal disilicides. In this study, a pressure-temperature phase diagram of $CaSi_2$ is investigated by in-situ x-ray diffraction measurements at pressures up to 15 GPa and temperatures from 290 to 1300 K.

Experiment

Powder sample of $CaSi_2$ was compressed in a multianvil high-pressure apparatus, MAX80. X-ray diffraction measurements were carried out by an energy-dispersive method with a solid-state detector in AR-NE5C line.

Results

$CaSi_2$ has a trigonal structure with six Si corrugated layers in the unit cell [4] (denoted by Tr6 in the following) at ambient conditions. The in situ observation revealed that $CaSi_2$ has three high-pressure phases at the pressure ranging from 0 to 15 GPa and temperatures ranging from 290 to 1300 K, as shown in the figure. One is the phase that has a tetragonal structure [3] (denoted by Tet), which appeared in heating above 3 GPa. The second is the phase that has a trigonal structure with a Si corrugated layer in the unit cell [4] (denoted by Tr1), which appeared in compression at room temperauture. The last is the phase that has an AlB_2-like structure, in which Si honeycomb layers are slightly corrugated [4] (denoted by Hex), which appeared in heating at 14.4 GPa, the maximum pressure in this study. The Tr1-to-Tet transition on heating at pressures ranging from 8 to 11 GPa indicates that Tet phase is also a high-temperature phase of Tr1.

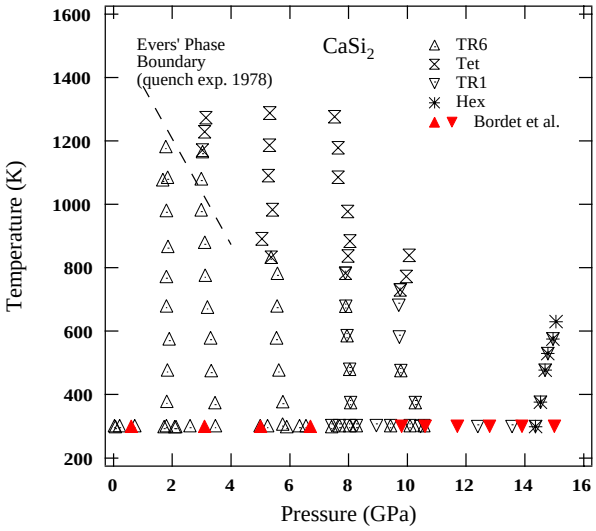

Fig. 1. Pressure-temperature diagram of $CaSi_2$.

References

[1] M. Imai et al., Phys. Rev. **B55**, 132 (1997).
[2] M. Imai et al., Phys. Rev. **B58**, 11922 (1998).
[3] M. S. Silverman et al., J. Phys. Chem. **67**, 1919 (1963).
[4] P. Bordet et al. Phys. Rev. **B62**, 11392 (2000).

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