M108

High-pressure polytypes of MgC_2 predicted by first-principles calculations

(Tohoku Univ.) Bin Wen, (Tohoku Univ.) Seiichi Takami, (Tohoku Univ.) Yoshiyuki Kawazoe, (Tohoku Univ.) Tadafumi Adschiri*

1. Introduction

As dicarbides have unique quantum properties and potential for use in superconductivity and thermoelectricity applications, they have attracted considerable attention in recent years. Among various alkaline-earth dicarbides, only MgC_2 has a unique *P42/mnm* crystal symmetry, whereas the other dicarbides, namely, BeC_2, CaC_2, SrC_2, and BaC_2, adopt an *I4/mmm* crystal symmetry[4]. Thus, MgC_2 may exhibit unique physical and chemical properties compared with the other alkaline-earth dicarbides.

2. Computational method

Three kinds of MgC_2 polytypes, namely, *P42/mnm*, CaC_2-like, and $SrSi_2$-like MgC_2, were considered in this study. The crystal lattice parameters and atom positions of these MgC_2 polytypes under pressure were optimized using density functional theory (DFT) based on a planewave pseudopotential technique implemented in the CASTEP package, and the enthalpies of the corresponding optimized structures were obtained.

3. Results and discussion

The relative phase stability of MgC_2 polytypes with respect to pressure can be evaluated by comparing the enthalpies[25], because no temperature effects were considered in this study. In particular, the MgC_2 polytype geometries were optimized under different pressures of up to 40 GPa using DFT, and the enthalpies of these optimized polytypes were obtained. The relationship between enthalpy and pressure is plotted in Figure 1 for various MgC_2 polytypes. As shown in this figure, when the pressure is below 7.5 GPa, the *P42/mnm* MgC_2 is energetically most stable. In the 7.5 to 20.5 GPa pressure range, the CaC_2-like MgC_2 becomes the most stable polytype. When the pressure is above 20.5 GPa, the $SrSi_2$-like MgC_2 becomes the most stable polytype. These results suggest that CaC_2-like and $SrSi_2$-like MgC_2 are two new high-pressure stable polytypes of MgC_2.

4. Conclusions

In summary, the pressure dependence of phase stability transformations of MgC_2 polytypes was determined using first-principles calculations. Our results showed that the relative stability order changes with increasing pressure. With increasing pressure, the most stable phase changes from *P42/mnm* MgC_2 to CaC_2-like MgC_2 to $SrSi_2$-like MgC_2, and the corresponding transformation pressures are 7.5 and 20.5 GPa.

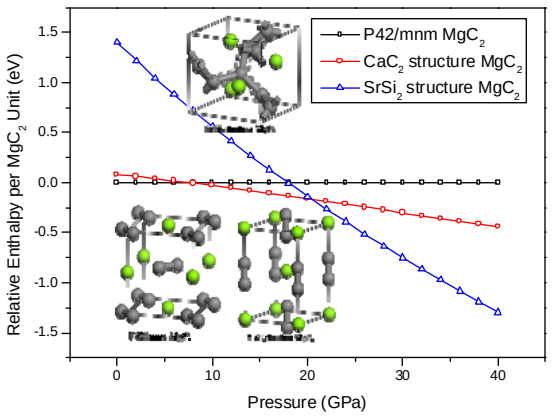

Figure 1. Relationship between enthalpy and pressure for *P42/mnm*, CaC_2-like, and $SrSi_2$-like MgC_2 determined from first-principles calculations.

* Corresponding authors. E-mail address: ajiri@tagen.tohoku.ac.jp