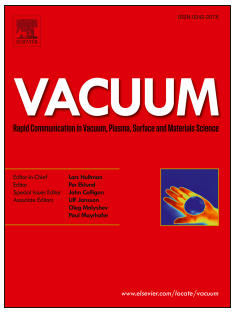
Accepted Manuscript



Comparative study on mechanical properties of three different SiC polytypes (3C, 4H and 6H) under high pressure: First-principle calculations

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PII: S0042-207X(18)30308-7

DOI: 10.1016/j.vacuum.2018.04.040

Reference: VAC 7945

To appear in: *Vacuum*

Received Date: 26 February 2018

Revised Date: 23 April 2018

Accepted Date: 26 April 2018

Please cite this article as: Peyvaste I, Alahyarizadeh G, Minuchehr A, Aghaie M, Comparative study on mechanical properties of three different SiC polytypes (3C, 4H and 6H) under high pressure: First-principle calculations, *Vacuum* (2018), doi: 10.1016/j.vacuum.2018.04.040.

Comparative study on mechanical properties of three different SiC polytypes (3C, 4H and 6H) under high pressure: first-principle calculations

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Abstract

A comparative study on the mechanical properties of three different SiC polytypes (3C, 4H, and 6H) under ambient and high pressures was conducted through first-principles calculations based on DFT. Two exchange correlation functions, namely, GGA, and LDA, were used to study the pressure-dependent mechanical properties of different SiC polytypes. The first computed results at ambient conditions indicated the GGA results were in closer agreement with the experimental results than LDA results. The superiority of GGA was ascribed to its accurate calculation based on electronic density and its gradient as a function of exchange correlation energy. The pressure-dependent behavior of the unit cell volume of 3C-SiC was investigated for first time which showed that the GGA approximation achieved accurate experimental data. The estimated elastic parameters of the SiC polytypes also exhibited high bulk and shear moduli, which reflected the high hardness properties of these materials. The mechanical stability of the three considered SiC structures under high pressure were investigated by using the well-known Born stability criteria, which showed that the three considered SiC structures were mechanically stable. The phase transitions of the three considered SiC to rock salt structures under high pressure were computed by LDA and GGA.

Keywords: SiC polytypes; mechanical properties; first-principles calculations; high pressure.