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Theoretical investigations on the structural, lattice dynamical and thermodynamic properties of XC (X = Si, Ge, Sn)

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ABSTRACT

First-principles calculations, which is based on the plane-wave pseudopotential approach to the density functional perturbation theory within the local density approximation, have been performed to investigate the structural, lattice dynamical, and thermodynamic properties of SiC, GeC, and SnC. The results of ground state parameters, phase transition pressure and phonon dispersion are compared and agree well with the experimental and theoretical data in the previous literature. The obtained phonon frequencies at the zone-center are analyzed. We also used the phonon density of states and quasiharmonic approximation to calculate and predict some thermodynamic properties such as entropy, heat capacity, internal energy, and phonon free energy of SiC, GeC, and SnC in B3 phase.

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1. Introduction

In recent years, IV–IV ground compounds such as SiC, GeC, and SnC have attracted both scientific and technological interest. Due to their good chemical stability, wide band gap, high hardness, high stiffness, high melting point and high thermal conductivity, they are considered to be a promising material for electronic and optical device. It is necessary to study their fundamental properties: lattice constants, bulk modulus, structural stability, electronic structure, and lattice dynamics.

Yoshida et al. [1] used X-ray diffraction measurements in static diamond-anvil cell (DAC) and investigated that the pressure-induced phase transition of SiC from B3 to B1 structure occurred at 100 GPa or higher. Some theoretical group also studied the phase transition of SiC using different methods [2–8]. These theoretical studies presented the critical pressure of SiC from B3 to B1 structure to be around 60 GPa. Hao et al. [8] also investigated the critical pressure of GeC and SnC to be around 89 and 32 GPa, respectively, and they also calculated the electronic, elastic and optical properties under high pressure using first-principles calculations based on the density functional theory with the plane wave. Pandey et al. [9] studied the structural stability, electronic, and optical properties of GeC and SnC at ambient pressure using a linear combination of atomic orbital approach. They presented the band gap from indirect to direct from SiC to GeC to SnC. Khenata et al. [10,11] investigated the structural and electronic, and optical properties of SiC, GeC, and SnC using the full potential linear augmented plane wave (FP-LAPW) method. Sekkal and Zaoui [12] studied the structural and thermodynamic properties of GeC in B3 structure using an MD method. They predicted Debye temperature, thermal expansion, heat capacity, and Grüneisen parameter of GeC at zero pressure. Feldman et al. [13] experimentally investigated the dynamics property of SiC using Raman scattering measurements. They presented the phonon dispersion curves of SiC. Karch et al. [14,15] calculated phonon frequencies along the stacking direction of SiC using the self-consistent study, they found only small differences to Raman scattering measurements. Wang et al. [16] calculated the pressure dependence of Born effective charges, dielectric constant, and lattice dynamics in SiC using the linearized augmented plane wave (LAPW) method.

A lot of studies have been carried out to calculate the structure and electronic properties of the B3 XC (X = Si, Ge, Sn), but many of their dynamical and thermodynamic properties are still not well established. To the best of our knowledge, there are no theoretical or experimental works exploring lattice dynamics properties of GeC, SnC and phonon contribution to the phonon free energy ΔF, the internal energy ΔE and the entropy S. Therefore, the aim of this work is to clarify the dynamical and thermodynamic properties of the XC (X = Si, Ge, Sn) in B3 phase.

The paper is organized as follows. In Section 1, we introduced the research progress briefly. In Section 2, we describe the computational method used in this work. We present our results and discussions in Section 3. Finally, a summary of the work is given in Section 4.

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Table 1
Calculated lattice constants (a in Å), bulk modulus (B_0 in Mbar) and its first pressure derivative (B_0') are compared to other theoretical calculations and experiments.

Lattice constant (Å)	B_0 (Mbar)	B_0'
SiC		
ZB		
This work 4.35	2.31	3.967
Experiment 4.36 [29]	2.25 [30]	–
Other works, 4.30 [7], 4.363 [8], 4.40 [9],	2.27 [7], 2.116 [8], 2.06 [9],	3.79 [8], 5.3 [9],
4.34 [10], 4.40 [11], 4.30 [12],	2.28 [10], 2.15 [11], 2.25 [12],	4.02 [10], 3.70 [11],
4.28 [26], 4.33 [27],4.32 [31],	2.45 [26], 2.29 [27], 2.25 [31],	3.90 [12], 3.94 [26],
4.35 [32]	2.22 [32]	4.11 [31], 3.8 [32]
RS		
This work 4.04	2.56	4.39
Other works 4.03 [2], 3.97 [7], 4.04 [8],	2.666 [7], 2.435 [8], 2.30 [10],	4.64 [7], 5.5 [10],
4.03 [10], 4.13 [12]	1.62 [12]	4.36 [12]
GeC		
ZB		
This work 4.59	2.01	4.17
Other works 4.589 [8], 4.61 [9],	1.75 [8], 1.81 [9],	4.2 [9], 3.73 [10],
4.54 [10], 4.62 [11],	2.03 [10], 2.00 [11],	4.15 [11], 3.45 [12],
4.43 [12], 4.49 [26],	1.88 [12], 2.18 [26],	
4.53 [27]	1.88 [27]	
RS		
This work 4.32	1.81	4.52
Other works 4.359 [8], 4.33 [10], 4.25 [12]	1.74 [8], 2.00 [10], 1.33 [12]	3.29 [10], 4.42 [12]
SnC		
ZB		
This work 5.13	1.17	4.24
Other works 5.113 [8], 5.17 [9], 5 [10],	1.198 [8], 1.19 [9], 1.47 [10],	4.3 [9], 4.51 [10], 4.31 [11]
5.10 [11], 4.84 [27]	1.25 [11], 1.33 [28]	
RS		
This work 4.72	1.59	4.39
Other works 4.829 [8], 4.70 [10]	1.346 [8], 1.66 [10]	4.7 [10]

2. Computational details

The ABINIT code [17–19], which is based on the plane-wave pseudopotential approach in the framework of the functional theory (DFT) and the density functional perturbation theory (DFPT), has been applied to calculate the structural, dynamical and thermodynamic properties of XC (X = Si, Ge, Sn) in B3 phase. The exchange-correlation term has been considered within the local density approximation (LDA). The norm-conserving local density approximation pseudopotentials of C, Si, Ge, and Sn are generated in the scheme of Troullier and Martins [20], which come from the ABINIT web site. Troullier and Martins pseudopotentials describe the interaction between the nuclei and core electrons and valence electrons. Per primitive unit cell contains two atoms in the ab initio calculations. To obtain the ground-state parameters, the B3 structures of SiC, GeC and SnC are first optimized by using a Broyden–Fletcher–Goldfarb–Shanno (BFGS) procedure [21]. An $8 \times 8 \times 8$ Monkhorst–Pack [22] grid is chosen for k-grid samplings in the Brillouin zone. The plane-wave kinetic energy cutoff of 40 hartree is set to guarantee the total energy errors within 0.0005 hartree in all the calculations. Convergence tests prove that the Brillouin zone sampling and the kinetic energy cutoff are reliable to guarantee excellent convergence. Phonon frequencies are calculated using the DFPT linear-response method [23,24]. The thermodynamic properties are calculated using the phonon density of states and quasiharmonic approximation.

3. Results and discussions

3.1. Structural properties

The equilibrium lattice parameters a, bulk modulus B_0, and their pressure derivatives of bulk modulus B_0' were calculated by means of fitting Murnaghan's [25] equation of state (EOS) to total energies versus volume. We summarized our results and the experimental and other theoretical values in the B1 and B3 phase in Table 1. It can be clearly seen that the calculated structural parameters are in excellent agreement with experimental values and other theoretical ones. The slight underestimation in the equilibrium lattice parameter is a common feature with LDA calculations. The calculated bulk modulus decreases from SiC to SnC, suggesting that the compressibility increases from SiC to SnC. We note that the anion atoms are the same in the three compounds, the cation atoms size are different. The different size of the cation atoms could be the responsible for the lattice constant increasing from SiC to SnC.

Table 2
Calculated phase transition pressure from B3 to B1 phase.

Material	Reference	Pt (GPa)
SiC	Present (LDA)	62
	Experimental [1]	100
	Theory (LDA) [2]	66.5
	Theory (LDA) [3]	65.3
	Theory (GGA) [4]	63
	Theory (LDA) [5]	92
	Theory (LDA) [6]	63
	Theory (GGA) [7]	75.4
	Theory (LDA) [8]	65.1
GeC	Present (LDA)	87
	Theory (LDA) [8]	89.4
SnC	Present (LDA)	33
	Theory (LDA) [8]	32.5

We calculated the phase transition pressure at $T = 0$ K using the usual method of equal enthalpies, i.e., the enthalpy as the function of pressure, $H = E + PV$. The enthalpy as a function of pressure for SiC, GeC, and SnC in B3 and B1 phases is illustrated in Fig. 1. Our results of phase transition pressures from B3 to B1 structure of SiC, GeC, and SnC are tabulated in Table 2. The calculated phase transition pressure of SiC is similar to

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