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Elastic, vibrational and thermodynamic properties of α−Sn based group IV semiconductors and GeC under pressure

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ABSTRACT

We present first-principles calculations of the structural, elastic, vibrational and thermodynamic properties of SnSi, SnGe, SnC and GeC. We employ the density-functional perturbation theory (DFPT) within the local density approximation in conjunction with the quasi-harmonic approximation. The calculated lattice parameters, which are obtained by minimizing the total energy, are in the range of those reported in the literature for the binary compounds and in good agreement with the measured ones for the elemental components. Our results for the elastic properties show that c_{44} softens as pressure increases for SnSi and SnGe. The phonon spectra, the density of states and the Born effective charge at zero pressure are calculated and the phonon frequencies are positive. A pressure induced soft transverse acoustic phonon mode is identified at the zone boundary X point of the Brillouin zone at pressure of 12.95 and 12.45 GPa for SnSi and SnGe respectively. The linear expansion coefficient for the elemental components is calculated and compared to experiment. The temperature and pressure dependence of the thermal expansion, the overall Grüneisen parameter, the bulk modulus and the heat capacity is predicted. The thermal expansion coefficient decreases with increasing pressure and does not show any negative behavior for GeC and this is due to the positive transverse acoustic mode Grüneisen parameters. Our results for Sn_xGe_{1-x} alloys using the supercell method indicate that the variation of the Grüneisen parameter and the thermal expansion with concentration has the same trend and the bulk modulus softens.

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1. Introduction

Silicon and germanium are the most technologically developed electronic materials. The semiconductor alloys based on group-IV elements such as SiC, SiGe, SnC and GeC are attractive for band gap and strain engineering of heterostructures [1,2] and have a number of remarkable properties which set them apart from other III–V and II–VI compounds, and make them particularity worthy of study. Under ambient conditions, Si, Ge and C crystallize in the diamond structure, while α−Sn is stable at low temperature below T=286 K [3,4]. The lattice mismatch between these elements is very high, about 15% between Ge and α−Sn, and 59% between C and Ge, the difference in electronegativity is important, and the solubility is very low [5]. Therefore, careful optimization of the growth parameters is required to obtain a material suitable for device applications. Despite the large lattice mismatch between the elemental constituents, SnGe films have been successfully grown on different substrates [6–13]. In the past, investigations of structural, electronic and optical properties of SnSi, SnGe, SnC and GeC and their alloys have been carried out by many groups [14–27]. All of these studies show that GeC, like SiC, is a wide gap semiconductor with an indirect band gap, but SnC and SnGe are narrow gap semiconductors. Unfortunately, there are only few reported works on the lattice dynamics and the thermodynamic properties of the above-cited materials [28–33].

The lattice vibrations play an important role for materials modeling and their behavior under pressure provides useful information regarding structural instabilities and phase transformation. It can be used to derive thermodynamic properties within the quasi-harmonic approximation, such as specific heat and thermal expansion. Therefore, a complete knowledge of the vibrational spectra is necessary for the investigation of the thermodynamic properties.

The aim of the present work is to present first principles calculation of the elastic constants, lattice dynamics and some thermodynamics properties of SnX (X=C, Ge, Si) and GeC under pressure by employing the plane wave pseudopotential method within density functional theory and the linear response technique. Furthermore, and in order to judge the reliability of our calculations, we evaluated the structural, the elastic properties and the linear thermal expansion of the elemental components (α−Sn,

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Si, Ge and C) for which extensive theoretical and experimental studies are available in the literature. The remainder of this paper is organized as follows: in Section 2 the details of the calculations are described. The results for the structural, elastic, vibrational and thermodynamic properties are presented and discussed in Section 3. Finally, a conclusion is given in Section 4.

2. Details of the calculations

The calculations are done using both the pseudopotential plane wave methods in the framework of the density functional theory (DFT) [34] within the local density approximation (LDA) using the Ceperley–Alder [35] and Perdew–Wang [36] form for the exchange–correlation energy according to Teter Pade parametrization [37]. Norm conserving Troullier and Martins pseudopotential (NCPP) generated with the Fritz-Haber-Institute pseudopotential program (FHI98PP) [38,39] is used for all atoms of the studied semiconductors as supplied in the ABINIT code [40,41]. The states C ($2s^2 2p^2$), Si ($3s^2 3p^2$), Ge ($4s^2 4p^2$) and Sn ($5s^2 5p^2$) are treated as valence states.

The elastic constants, phonon dispersion curves and phonon density of states are calculated by using density functional perturbation theory [42–45] as implemented in the ABINIT code. Brillouin zone integration was performed by k-point sampling with special points obtained by using the standard special k-points technique of Monkhorst and Pack (MP) [46]. In this work, an $8\times8\times8$ MP mesh and a cutoff energy of 80 Ry are used for all compounds.

We have also used the projector augmented wave method (PAW) [47] as implemented in the ab initio total energy and molecular dynamics program VASP (Vienna ab initio simulation program) developed at the Institut für Material physik of the Universität Wien [48,49]. The interaction between ions and valence electrons is described by the projector augmented wave potential and a plane wave energy cutoff approximately 25% above the default value and $4\times4\times4$ MP k-points mesh to ensure a good convergence. The phonon spectra are calculated using the supercell approach as implemented in the phonopy package [50,51] using a $2\times2\times2$ conventional unit cells (64 atom supercell).

3. Results

3.1. Structural properties

The cubic lattice is characterized by the lattice parameter a_0, to obtain its ground state value the total energy per primitive cell as a function of volume is calculated and then fitted to the Vinet equation of state (EOS) [52]. The calculated structural parameters for the studied binary compounds are listed in Table 1, together with those of the elemental components obtained in the cubic phase. We note that the elemental components of the compounds considered here (i.e. C, Si, Ge, $\alpha-$Sn) have a diamond structure [53], while SnX (X=Si, Ge, $\alpha-$Sn) and GeC are treated in the zinc blende one. For the elemental components, for which experimental data have been reported, our calculated values of the structural parameters are in good agreement with the measured ones at 300 K.

The cubic lattice constant for the alloy AB is also estimated using Végard's law: $a_{AB}=(1/2)[a_A+a_B]$, and the obtained values (see Table 1) are very close to those obtained by energy minimization. Thus, we conclude that Végard's law is respected for these compounds. The calculated bulk modulus of SnSi, SnGe, SnC and GeC are 68, 60.36, 156.67 and 200 GPa, respectively. Furthermore, the application of the empirical formula $B_0=1761d^{-3.5}$ of Cohen [54] with the calculated nearest neighbor distances gives the values of 66.70, 63.46, 128.40 and 173.83 GPa, respectively. Our predicted values for the first two compounds, i.e. SnSi and SnGe, are similar to those determined by Cohen's formula, while for the other two compounds the agreement is poor. However, the application of the relation of $B=1972d^{-3.5}$ results the values of 75.50, 71.08, 143.79 and 197.44 GPa for SnSi, SnGe, SnC and GeC, respectively.

Table 1
Structural parameters; lattice parameter a_0 in (Å), bulk modulus B in (GPa) and its pressure derivative B' for zinc blende structures of SnX (X=Si, Ge, Sn), GeC and the constituent elements. Experimental data are given in parentheses (the values in bracket are calculated or estimated).

Compound	a_0	B	B'	$a_{AB}=(a_A+a_B)/2$
SnSi	5.89	67.87	4.62	5.87
Others	5.95[a], 5.91[b]	63[a], 65.3[b]	4.60[b]	
SnGe	5.97	60.26	4.75	5.96
Others	6.05[a],6.004[b], 6.09[c]	56[a], 57.1[b],54[d]	4.725[b],5.8[h],5.03[c]	
	6.09[d],6.20[e]	53[c],62.7[h],54[d]	6.8[c],6.9[e],4.78[i]	
	4.22[h],6.21[i]	53[e],46.32[i]	5.03[d]	
SnC	4.88	156.48	4.21	4.94
Others	4.83[a],4.96[b], 5[c]	133[a], 142.3[b], 147[c]	4.40[b], 4.51[c], 4.31[c]	
	5.10[c],5.005[d],5.17[f]	125[c],147[d], 119[f]	4.51[d],4.3[f]	
	5.00[g]	142[g]	4.68[g]	
GeC	4.48	200.36	4.13	4.54
Others	4.51[a], 4.50[b],4.54[c]	188[a], 194.6[b], 200[c]	4.179[b], 3.73[c], 3.73[d]	
	4.54[d], 4.61[f],4.49[j]	203[d], 181[f],226.3[j]	4.2[f],4.01[g]	
	4.53[g], 4.43[k], 4.60[l]	200[g], 188[k], 173[l]	3.45[k], 4.458[l]	
C	3.52 (3.56)[m]	465.32 (452)[m]	3.61 (4.0)[n]	
Ge	5.57 (5.65)[o]	75.21 (74.7)[o]	4.61 (4.55)[a5]	
Si	5.38 (5.43)[o]	96.28 (97.84)[o]	4.24 (4.24)[o]	
Sn	6.37[p], 6.479[q] (6.48)[o]	48.7[p], 45.46[q] (42.5)[o]	4.76[p], 4.78[q] [4.55][o]	

[a] Ref. [28].
[b] Ref. [56].
[c] Ref. [23].
[d] Ref. [22].
[e] Ref. [16].
[f] Ref. [26].
[g] Ref. [20].
[h] Ref. [21].
[i] Ref. [55].
[j] Ref. [57].
[k] Ref. [29].
[l] Ref. [24].
[m] Ref. [58].
[n] Ref. [59].
[o] Ref. [53].
[p] Calculated using the NCPP method.
[q] Calculated using the PAW method.

3.2. Elastic properties

The elastic constants of solids provide a link between the mechanical and dynamical behaviors of crystals, and give important information concerning the nature of the forces operating in solids. Crystal with cubic symmetry has only three distinct non-vanishing elastic constants namely c_{11}, c_{12} and c_{44}. The calculated elastic constants are listed in Table 2 together with the available experimental data and results of the other calculations. All the calculated elastic constants in Table 2 satisfy the mechanical stability criteria in cubic crystal [60]; $c_{11}-c_{12}>0$; $c_{44}>0$; $B>0$. From Tables 1 and 2, we can see that the calculated value of the

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