

Structural, electronic and energetic properties of silicon carbon alloys

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Received 7 January 2006; received in revised form 9 April 2006; accepted 18 May 2006

Abstract

We studied the influence of alloying on the structural and electronic properties of the unrelaxed and relaxed $\text{Si}_{1-y}\text{C}_y$ random alloys by means of ab initio theoretical calculations using two methods: (i) a supercell approach in connection with the plane-wave pseudopotential method; (ii) the full-potential augmented plane-wave plus local orbitals (APW + lo) method. The first method is used to obtain the relaxed atomic structure. The relaxed atomic positions obtained by pseudopotential calculations were used to calculate the band structure via the second method. The local density approximation was used for the exchange and correlation energy density functional. We investigated the lattice parameters and band gap energies. We found that a quite smaller gap appears in the neighborhood of $y = 0.03125$ concentration of C atoms. The band gap shows a large anomalous bowing and is strongly composition dependent. The electron densities of states for the unrelaxed and relaxed $\text{Si}_{1-y}\text{C}_y$ are also presented. A model structure of 16- and 32-atom supercells is used. The calculated formation enthalpy and individual energy contributions for $y = 0.5$ show that the instability of $\text{Si}_{1-y}\text{C}_y$ alloys is dominated by the largest term of the elastic energy.

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PACS: 31.15.Ew; 71.15.Mb; 71.15.Dx; 71.20.Mq; 61.66.Dk

Keywords: Density functional theory; Local density approximation; Pseudopotential method; Elemental semiconductors; Alloys

1. Introduction

In view of their technological promise, $\text{Si}_{1-y}\text{C}_y$ alloys have attracted increasing research interest in the last few years. Although they are members of the binary group-IV alloys family, they have remarkable properties, which sets them apart from other binary alloys, such as $\text{Ge}_{1-y}\text{Si}_y$ [1,2]. These alloys containing carbon exhibit both physical and chemical properties that differ significantly from the general trends of the group-IV family.

The quest for realization of such materials is motivated by the desire to manipulate the band gap of silicon, which can be achieved through alloying or by creating strained-layer superlattices (SLs). A prototypical and extensively studied system is silicon–germanium ($\text{Si}_y\text{Ge}_{1-y}$) alloys [1,2]

whose band gap can be varied monotonically from 0.66 to 1.12 eV as y increases from 0.0 to 1.0. Another interesting case is the binary silicon–carbon ($\text{Si}_{1-y}\text{C}_y$) system. Various groups [3,4] reported that the inclusion of C in pseudomorphic $\text{Si}_{1-y}\text{Ge}_y$ layers on Si substrates can compensate for the compressive strain. The solubility of carbon in silicon under equilibrium conditions is extremely small because of the huge lattice constant mismatch and the cost in elastic energy (strained bonds) as carbon is incorporated into the lattice. Therefore, experimental efforts to overcome this obstacle have been based on non-equilibrium methods, such as growth of films by molecular beam epitaxy [5,6] and chemical vapor deposition [7], which exploit the less constrained environment and the higher atomic mobility on surfaces. The discussion of the electronic properties of $\text{Si}_{1-y}\text{C}_y$ alloys has been quite controversial. The possibility that incorporation of carbon, which in the diamond bulk phase has a larger band gap

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than Si, might yield a wide-band-gap Si-based material is appealing. It is, however, not obvious that C incorporation will yield the desired effect.

Extensive theoretical studies were reported [8–13], Demkov and Sankey [8] pointed out that adding carbon to silicon would lower the gap more and more up to a concentration of about 10% before the slope changes sign and the gap begins to increase. They attributed this behavior to the large chemistry difference between carbon and silicon. Our recently published work supported this result [13]. Many efforts, both theoretical and experimental, have been performed to characterize the energy band structure of $\text{Si}_{1-y}\text{C}_y$ alloys [14–22]. So far, the understanding of the electronic energy band structures of such materials is limited. In contrast to the earlier experimental results [3,4,23] which assumed that the structural parameters of the binary alloys obey the Vegard's law, Kelires [24], using a Monte Carlo method, reported that the lattice structural parameters of the $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ alloy present strong deviations from the linear behavior.

We previously published the results of a study on $\text{Si}_{1-y}\text{C}_y$ alloys [13] using a small 8-atom supercell; in the present work we extend our study to 32-atom supercells with the aim of explaining the effect of the size of the cell on the structural and electronic properties.

In this paper, the first-principles full-potential linearized augmented plane wave plus local orbital (APW+lo) calculation is performed for $\text{Si}_{1-y}\text{C}_y$ alloys, with several C concentrations, to investigate the dependence of the band gap on the concentrations. The remainder of the paper is organized as follows. In Section 2, we describe the crystal structure model and the methods of calculation. The results obtained for $\text{Si}_{1-y}\text{C}_y$ alloys with several C concentrations are presented in Section 3. Discussions and summary are made in Section 4.

2. Calculations

The local density approximation (LDA) was employed to calculate total energies and electronic structures in a manner similar to our previous work [13]. The electronic configurations for Si and C are $\text{Ne } 3s^2 3p^2$ and $\text{He } 2s^2 2p^2$, respectively. In the following calculation, the subshells of the noble gas cores have been distinguished from the subshells of valence electrons given explicitly. All calculations are performed using the Vienna package WIEN2K [25]. This is an implementation of a hybrid full-potential (linear) augmented plane-wave plus local orbitals (L/APW+lo) method within the density-functional theory [26,27]. This new approach is shown to reproduce the accurate results of the L/APW method, but using a smaller basis set size. Due to the smaller basis set and faster matrix setup, APW+lo offers a shorter runtime and uses less memory than L/APW. The effects of using APW+lo are greatest for calculations with a large ratio of basis functions to atoms, e.g., for open crystal structures, surfaces and molecules on surfaces [28].

The APW+lo method expands the Kohn–Sham orbitals in atomic-like orbitals inside the atomic muffin-tin (MT) spheres and plane waves in the interstitial region. The details of the method have been described in the literature [28–30]. The basis set inside each MT sphere is split into core and valence subsets. The core states are treated within the spherical part of the potential only and are assumed to have a spherically symmetric charge density totally confined inside the MT spheres. The valence part is treated within a potential expanded into spherical harmonics up to $l = 4$. The valence wave functions inside the spheres are expanded up to $l = 10$. A plane-wave expansion with $R_{\text{MT}}-K_{\text{MAX}}$ equal to 8, and k sampling with a $8k$ -point mesh in the full Brillouin zone turns out to be satisfactory. The k integration over the Brillouin zone is performed using the Monkhorst and Pack mesh [31]. All of the calculations are carried out at the theoretical equilibrium lattice constants.

We take the Perdew–Wang LDA [32] for the exchange–correlation potentials. The self-consistent calculations are considered to be converged only when the calculated total energy of the crystal converged to less than 1 mRy. The choice of the particular (and different) MT radii for the various atoms in the compounds shows small differences that do not affect our results. We have adopted the values of 1.9 and 1.8 bohr for silicon and carbon, respectively, as the MT radii. We compute lattice constants and bulk moduli by fitting the total energy versus volume curves to the equation of states.

The supercell approach is adopted to model the considered $\text{Si}_{1-y}\text{C}_y$ alloys. We used a 32-atom $\text{Si}_{32-n}\text{C}_n$ supercell. For a given number $n = 0, \dots, 4$ of C atoms, different atomic configurations have been optimized structurally. However, it is impossible to treat all different atomic configurations. Therefore, for a given number n of C atoms, we usually study only a small number of different configurations in which the C atoms are not really randomly distributed.

Rather, we choose a more appropriate strategy. We begin with a maximum Si–C clustered alloy, then we sequentially move the C atoms out of the cluster. For instance, in the $n = 4$ case, the first configuration corresponds to one atom of Si bounded to four atoms of C, and the last configuration corresponds to one atom of Si bounded to only one atom of C (the Carbon distances are as far as possible). For each configuration and each atomic number n , the fundamental physical properties (total energy and band gap) are determined.

The positions of atoms in the relaxed $\text{Si}_{1-y}\text{C}_y$ alloys are determined by minimizing the total energy of the system. We used ab initio plane-wave pseudopotential calculation as implemented in the PWSCF package to obtain the geometrically relaxed atomic structure of random 32-atom supercells for four different configurations of the $\text{Si}_{1-y}\text{C}_y$ alloys with carbon concentrations y of 3.125, 6.25, 9.375 and 12.5%. Due to the strong p pseudopotential of carbon (characterized by highly localized orbitals (C 2s and

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