States of silicon nanoclusters containing carbon impurities

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The structural and electronic states of defective complexes in the Si_{29} cluster with the participation of carbon and hydrogen atoms were determined by the method of non-conventional strong binding (MNSB) in combination with the method of molecular dynamics. It is shown that carbon atoms in silicon clusters form a bridge bond with two silicon atoms and localized in a hexagonal position at the center of the cell, forming a defect of the $Si_{29}:C_i$ type. The introduction of hydrogen into a silicon cluster results in the formation of a defective C_i-H-Si complex and a decrease of binding energy of the $Si_{29}:C_i$ defect. Based on the calculations, it was found that presence of leads to carbon gives shallow levels in the band gap of nano-silicon, and the defective carbon-hydrogen complex in a hydrogenated cluster, depending on the charge state of the defective complex. Moreover this exhibits both deep and shallow levels.

Keywords: MD and MNSB methods, silicon nano-clusters, hydrogenated cluster, structural defects, *ab initio* methods, carbon and hydrogen atoms, spatial structure, shallow and deep levels.

1. Introduction

In recent years, the need to find new materials for nano-electronics has stimulated active research into the methods of adjusting the properties of semiconductors via the formation of low-dimensional nanoclusters in their matrix. Unique properties of nanoclusters, such as a strong dependence of their electronic structures on size, composition, and geometric parameters, which provides an opportunity to model the needed device characteristics, makes them viable candidates for use in materials of this kind.

Clusters may contain atoms of introduced and related impurities, atoms of intrinsic components, and intrinsic point defects of the crystal lattice. Since single-crystal silicon is the base material of modern semiconductor electronics with related impurities (e.g., oxygen, carbon and hydrogen, which tend to form various low-dimensional structural defect complexes) present in the matrix, these impurities may exert a considerable influence on the structure of silicon clusters, altering their properties and electronic states. State changes of clusters may be predicted by modeling the structure of silicon nanoclusters [1]. The majority of published studies in this field are focused on the application of different methods for examining the structure of clusters formed from intrinsic atoms without the inclusion of impurity defects. A complex approach (a combination of semi-empirical, *ab initio*, and other computational approaches) is needed to optimize the geometry and perform model calculations of the electronic structure of silicon clusters with related impurities. The aim of the present study is to calculate the structure and electronic states of silicon clusters containing carbon atoms with different charges and identify the influence of interstitial hydrogen atoms on the characteristics of a cluster with 29 silicon atoms by applying a combination of the methods of non-conventional strong binding and molecular dynamics.

2. Calculation procedure

Silicon nanosized dimerized and nondimerized hydrogenated (with dangling surface bonds neutralized by hydrogen atoms) clusters type $Si_{29}:C$, $Si_{29}H_{24}:C$, and $Si_{29}H_{36}:C$ were examined.

Let us consider first the process of formation of defects in single-crystal silicon involving carbon and hydrogen. Carbon is an uncontrolled impurity in Si, and its concentration in the Si matrix may reach $2 \cdot 10^{18}\,cm^{-3}$. It has been assumed that its presence in melt may affect only the structural perfection of grown single crystals and that this impurity is electrically neutral. However, it has recently been found that carbon interacting with related impurities (especially oxygen) may also affect the electrophysical material properties: suppress the formation of oxygen thermodonors and form carbon–oxygen CO_n-type complexes. Essential information regarding the state of impurity carbon in silicon has been derived from EPR data in [2,3]. Three types of pair-forming electrically active states of carbon have been identified: positively charged interstitial-site state C_i^+; neutral state C_i^0 that decomposes thermally at $65°C$; and pair $C_S - C_i$ that remains stable to $250°C$. The authors of [4,5] have also found that carbon is likely to be located at an interstitial site. The presence of

both oxygen and carbon in silicon under thermal treatment may stimulate the formation of associates as a result of precipitation of impurities from their supersaturated solid solutions with subsequent formation of various microdefects up to a concentration of $\sim 10^8-10^9\,\mathrm{cm}^{-3}$ with sizes of $\sim 60-80\,\mathrm{nm}$ [6]. These microdefects may be minimized by processing a crystal in the atmosphere of argon with added hydrogen. Processing in pure hydrogen leads to the formation of microdefects of a new type (hydrogen precipitate) that have a negative effect on the mechanical strength and oxidation stability of silicon. According to literature data, hydrogen atoms are located at interstitial sites of diamond-like semiconductors and form complex defects with an energy spectrum that is similar in nature to the one of hydrogen-like impurities, but differs in the impurity center symmetry from common hydrogen-like substitutional impurities [7]. The binding energy of hydrogen and silicon atoms is $\sim 2.0\,\mathrm{eV}$. An ionization energy this high makes it impossible for atomic hydrogen to manifest electrical activity. It is known that the properties of a silicon surface stabilize after saturation with hydrogen due to termination of dangling chemical bonds of silicon atoms. However, data on the behavior of hydrogen in silicon clusters at a varying concentration of impurity carbon are virtually lacking. The structure of formed clusters with carbon and hydrogen may be determined by modeling. It will be shown below that the use of combined techniques for examining the electronic structure of silicon clusters should allow one to model the optimized geometric structure of silicon clusters with carbon impurities and introduced hydrogen atoms based on the results of theoretical calculations.

A combination of the methods of non-conventional strong binding (NSB) [8,9], wherein the physical and chemical properties of bonds both between matrix atoms and between matrix and impurity atoms (including all the components of the total internal binding energy of the lattice) are taken into account, and molecular dynamics (MD) was used to calculate the cluster structure. In this context, the procedure of parameterization allows one to calculate the structural parameters both of a defect-free lattice and a crystal with point defects. The equilibrium cluster geometry was optimized using the MD method. We used the NSB method with a total energy functional that differs in form from energy functionals that are commonly used in the strong binding (SB) method. The expression for the NSB total energy functional may be written as follows [8]:

$$
\begin{aligned}
E_{tot} = & \sum_{\mu}\sum_{\nu>\mu}\frac{Z_{\mu}^{scr}(R_{\mu\nu})Z_{\nu}^{scr}(R_{\mu\nu})}{R_{\mu\nu}} \\
& + \sum_{\mu}\sum_{\nu>\mu}\frac{Q_{\mu}(R_{\mu\nu})Q_{\nu}(R_{\mu\nu})}{R_{\mu\nu}} \\
& + \sum_{\mu}\sum_{\nu>\mu}\sum_{i}\sum_{j}P_{\mu i,\nu j}H_{\mu i,\nu j} + \sum_{\mu}(E_{\mu}-E_{\mu}^0), \quad (1)
\end{aligned}
$$

where $R_{\mu\nu}$ is the internuclear distance, screened nuclear charge

$$
\begin{aligned}
Z_{\mu}^{scr} &= Z_{\mu}^{scr}(R_{\mu\nu}, \{N_{\mu i}^0\}) \\
&= Z_{\mu} - \sum_{i}N_{\mu i}^0\left[1 - a_{\mu i}\exp(-\alpha_{\mu i}R_{\mu\nu}/R_{\mu i}^0)\right], \quad (2)
\end{aligned}
$$

nonpoint ionic charge

$$
Q_{\mu} = Z_{\mu}^{scr}(R_{\mu\nu}, \{N_{\mu i}^0\}) - Z_{\mu}^{scr}(R_{\mu\nu}, \{N_{\mu i}\}), \quad (3)
$$

Z_{μ} is the charge of the μ-th nucleus (or nucleus plus core electrons); $R_{\mu i}^0 = n/\xi_{\mu i}^0$ is the most probable electron–nucleus distance, n and $\xi_{\mu i}^0$ are the principal quantum number and Slater exponents of the i-th atomic orbital (AO) centered at the μ-th nucleus; E_{μ}^0 and E_{μ} are the total energies of individual atoms in noninteracting and interacting systems characterized by sets of occupancy numbers $\{N_{\mu i}^0 \equiv P_{\mu i,\mu i}^0\}$ and $\{N_{\mu i} \equiv P_{\mu i,\mu i}\}$ (here, $P_{\mu i,\mu i}^0$ and $P_{\mu i,\mu i}$ are functions characterizing the degree of „point-likeness" of an electron cloud around a nucleus) and energies $\{E_{\mu i}^0\}$ and $\{E_{\mu i}\}$ of valence AOs, respectively; and α and a are fitting parameters. Atomic units are assumed here and elsewhere.

The first term in (1) represents the repulsion of screened nuclear charges of neutral atoms in the ground state. The second term in Eq. (1) may be nonzero even for a neutral atom.

AOs for a neutral diatomic molecule are assumed to be orthogonal, and matrix equation of the form

$$
\sum_{\nu i}(H_{\mu i,\nu j} - \varepsilon\delta_{\mu i,\nu j})C_{\nu j} = 0 \quad (4)
$$

is solved self-consistently to determine energy spectrum $\{\varepsilon_k\}$ and AO expansion coefficients $C_{\nu j}$ of molecular orbitals (MO) of the system, where $\delta_{\mu i,\nu j}$ is the perturbation potential in interaction of a μ-atomic orbital of an i-atom with a ν-atomic orbital of a j-atom.

In the NSB parameterization, the parameters of small clusters determined in *ab initio* calculations [10] are the base reference systems. The accuracy of calculation is ensured by correct parameterization of geometric and energy characteristics and spectroscopic energies of small systems performed with the use expression (1) for the total energy with its components being defined based on the individual parameters (AO energies and Slater exponents) of chemical elements.

The method of molecular dynamics was used to optimize the spatial structure of clusters. The MD method [11] relies on classical mechanics; more specifically, it is based on the numerical integration of Newtonian equations of motion [9]:

$$
m_i d^2\vec{r}_i/dt^2 = m_i\vec{a}_i = \vec{F}_i; \quad \vec{F}_i = dU/d\vec{r}_i, \quad (5)
$$

where m_i, $\vec{r}_i$, and $\vec{a}_i$ are the mass, the position, and the acceleration of the i-th particle, respectively; $\vec{F}_i$ is the force acting on the i-th particle from other particles; and U is
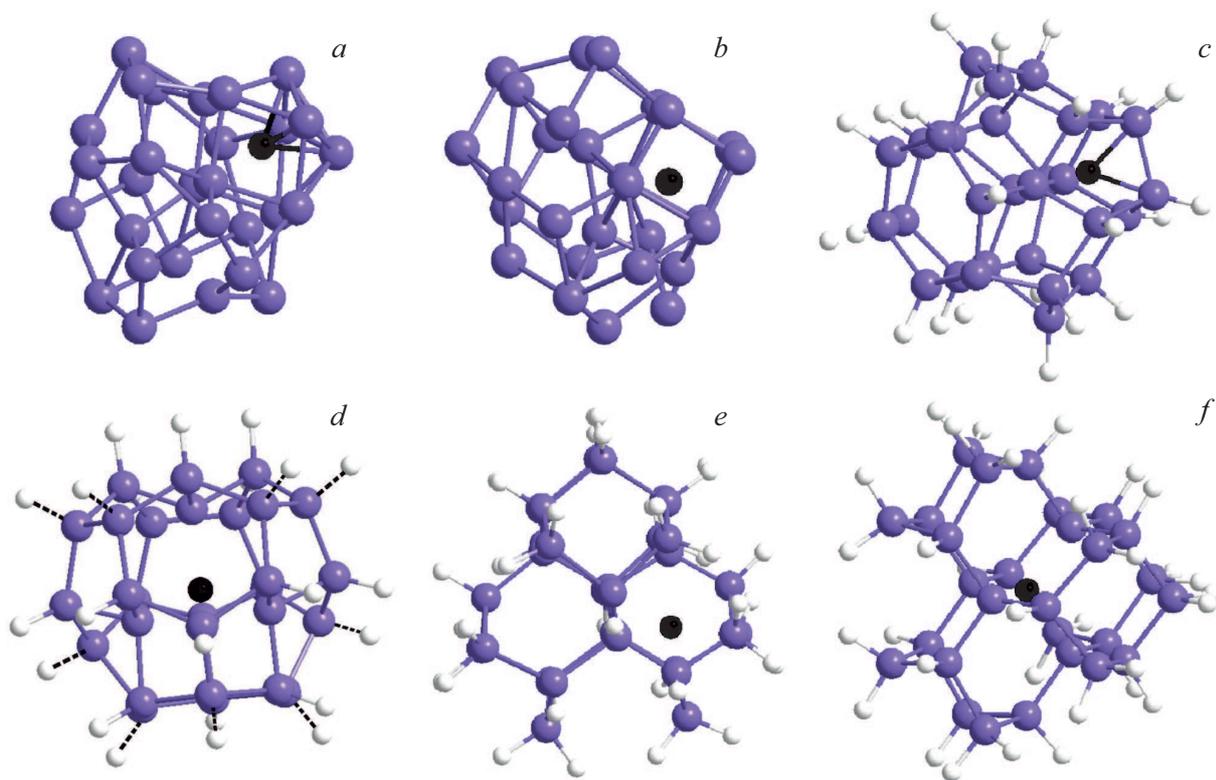
Figure 1. Spatial structure of C_i in different charge states: $Si_{29}:C_i(+)$ (a), $Si_{29}:C_i(-)$ (b), $Si_{29}H_{24}:C_i(+)$ (c), $Si_{29}H_{24}:C_i(-)$ (d), $Si_{29}H_{36}:C_i(+)$ (e), and $Si_{29}H_{36}:C_i(-)$ (f). Black dots in the figures denote carbon atoms, hydrogen atoms are colored light blue, and silicon atoms are colored blue; black dashed lines represent weak $Si-H$ bonds, which are a fraction of an angstrom longer than equilibrium $Si-H$ bonds. (A color version of the figure is provided in the online version of the paper).

the total potential energy of the system, which may be calculated using one of the approximate methods.

When performing a comparative analysis of the energy characteristics, one should take into account the fact that the total internal energy is underestimated and overestimated in calculations relying on semi-empirical strong binding methods and *ab initio* methods based on the density functional theory, respectively. The next step in approximation to the ideal state of an interacting system of many charged particles is the single-electron approximation (i.e., reduction of a many-electron problem to a single-electron one). While maintaining the accuracy of structural parameters of a system and a fairly close fit to energy characteristics, these simplifying approximations lead to systematic underestimation of the total internal energy [12]. The single-electron approximation is also applied in *ab initio* calculations of parameters and characteristics of a system of interacting atoms to correct nonphysical deviations of the calculated values, but the interaction of electrons involved in bond formation is taken into account twice. Consequently, the total internal energy is overestimated [9]. However, the accuracy of calculation of structural parameters is the same in the considered two modeling methods. Therefore, the use of a semi-empirical approach in computer modeling of the structure and certain key energy parameters of clusters,

the data for which are comparable to the results of *ab initio* calculations (e.g., the results reported in [10]), is entirely justified. At the same time, the complexity of parameterization and limited applicability of semi-empirical strong binding methods and the need to perform comparative analysis with widely used *ab initio* methods motivated us to turn to the ORCA software package for optimizing the structural and energy parameters of nanosized silicon clusters. Further studies were performed with the use of *ab initio* methods.

3. Results and discussion

3.1. Carbon defect centers in silicon clusters

Interstitial carbon atoms at different sites in a pure surface-dimerized $Si_{29}:C_i$ cluster and hydrogenated $Si_{29}H_{24}:C_i$ and $Si_{29}H_{36}:C_i$ clusters in positive and negative charge states of carbon were calculated initially for the modeling of structures (Fig. 1).

The presented spatial structures demonstrate that a carbon atom forms a bridge bond with two silicon atoms and is localized at an interstitial site (in what follows, this atom is denoted as C_i, and an impurity carbon atom occupying a silicon lattice site is denoted as C_s). In the modeled structures, a carbon atom is positioned either at a hexagonal
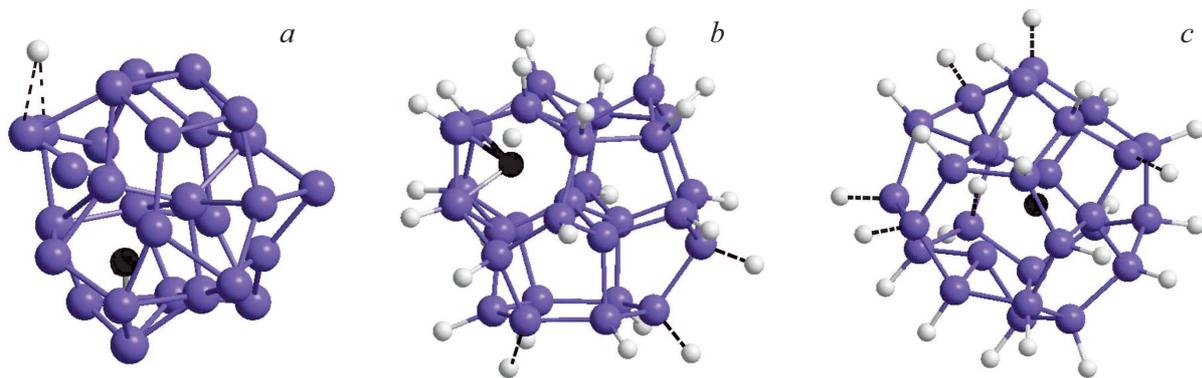
Figure 2. Spatial structure of charged states of defect complexes C_i-H: $Si_{29}:C_i$ (a), $Si_{29}H_{24}:(C_iH)^+$ (b), and $Si_{29}H_{24}:(C_iH)^-$ (c). Black dots in the figures denote carbon atoms, hydrogen atoms are colored light blue, and silicon atoms are colored blue; black dashed lines represent weak Si−H bonds, which are a fraction of an angstrom longer than equilibrium Si−H bonds.

Table 1. Energy parameters of impurity C_i in nanoclusters of pure Si_{29} and hydrogen-containing clusters $Si_{29}H_{24}$ and $Si_{29}H_{36}$

	Binding energy of carbon with a cluster, eV	E_{LUMO}, eV	E_{HOMO}, eV	E_g, eV
$Si_{29}:C_i(-)$	12.59	−8.61	−8.38	0.23
$Si_{29}:C_i(+)$	12.29	−8.26	−8.25	0.01
$Si_{29}H_{24}:C_i(-)$	7.51	−9.35	−9.06	0.29
$Si_{29}H_{24}:C_i(+)$	7.85	−8.86	−8.37	0.49
$Si_{29}H_{36}:C_i(-)$	6.61	−10.39	−8.96	1.43
$Si_{29}H_{36}:C_i(+)$	6.78	−9.53	−9.04	0.49

site at the center of the cell or as a substitutional impurity at the central T_d site.

The obtained results of calculation of energy parameters of clusters are listed in Table 1. It can be seen that the binding energy of a carbon atom with a silicon cluster is the most pronounced for a pure Si_{29} cluster with dangling orbitals on the surface. This is apparently attributable to the binding energy variation. Another confirmation is that negatively charged defect states are bound stronger to a carbon atom. The generalized formula for calculation of the band gap for clusters doped with carbon may be written in the following form:

$$E_g = E_{HOMO} - E_{LUMO}, \qquad (6)$$

where E_{HOMO} is the energy level lying below the conduction-band bottom of a cluster and closest to it and E_{LUMO} is the energy level lying above the valence-band top of a cluster and closest to it. Local levels induced by impurity carbon atoms in the band gap of a cluster exert an insignificant influence on the band gap edges.

This may be attributed to the fact that, first, interstitial impurities normally introduce shallow levels into the band gap and, second, a carbon atom is close to silicon in its energy characteristics and valence state. Therefore,

this impurity does not form deep local levels even at a substitutional site. Since s carbon atom in the lattice cell of a silicon nanoparticle has a significantly smaller covalent radius (0.771 Å) than matrix atoms (1.173 Å), it may maintain a certain charge state for a much longer period of time. This provides an advantage for an interstitial position of an impurity carbon atom in the matrix of silicon atoms, thus agreeing closely with the data from [4].

3.2. Carbon–hydrogen impurity centers in silicon clusters

It was found in the examination of literature data [2,4,13,14] that hydrogen is a stabilizing impurity in silicon. Let us consider its influence on silicon clusters containing carbon impurities. Complexes featuring individual hydrogen atoms in silicon and containing carbon atoms were identified in DLTS experiments [15–17]. It was demonstrated that a C_iH pair has a deep donor level $E_C - 0.16$ eV. It is assumed that, having captured an electron, a C_i-H complex [13,16] dissociates, changes its charge state [13,17], and then decomposes to a neutral state with an activation energy of 0.5 eV [17–19]. The calculated models of structures of silicon clusters associated with a C_i-H impurity are presented in Fig. 2.

The electronegativity of carbon is greater than that of silicon, but the electronic configuration of silicon in the vicinity of a C_i-H defect center may change from $3s^2 3p^2$ to $3s^3 p^3$ [14,20,21]. This is also associated with a weakly manifested transition of a silicon electron from a p^2 orbital to d, which leads to a change in the electron configuration of a C−H−Si complex. Thus, it was hypothesized that the structure of this complex is a hydrogen atom bond between substitutional C and an adjacent Si atom. The binding energy of neutral H−C was determined to be −1.17 eV, and this defect was found to be bistable. In positive and neutral charge states, H is located close to the C−Si bond center [20]; however, hydrogen in a negative state is positioned at the opposite side of this bond. An interstitial

Energy level diagram: Si29CH36_0

Si$_{29}$H$_{36}$: C$_i$

Energy level diagram: Si29CH1H36_0
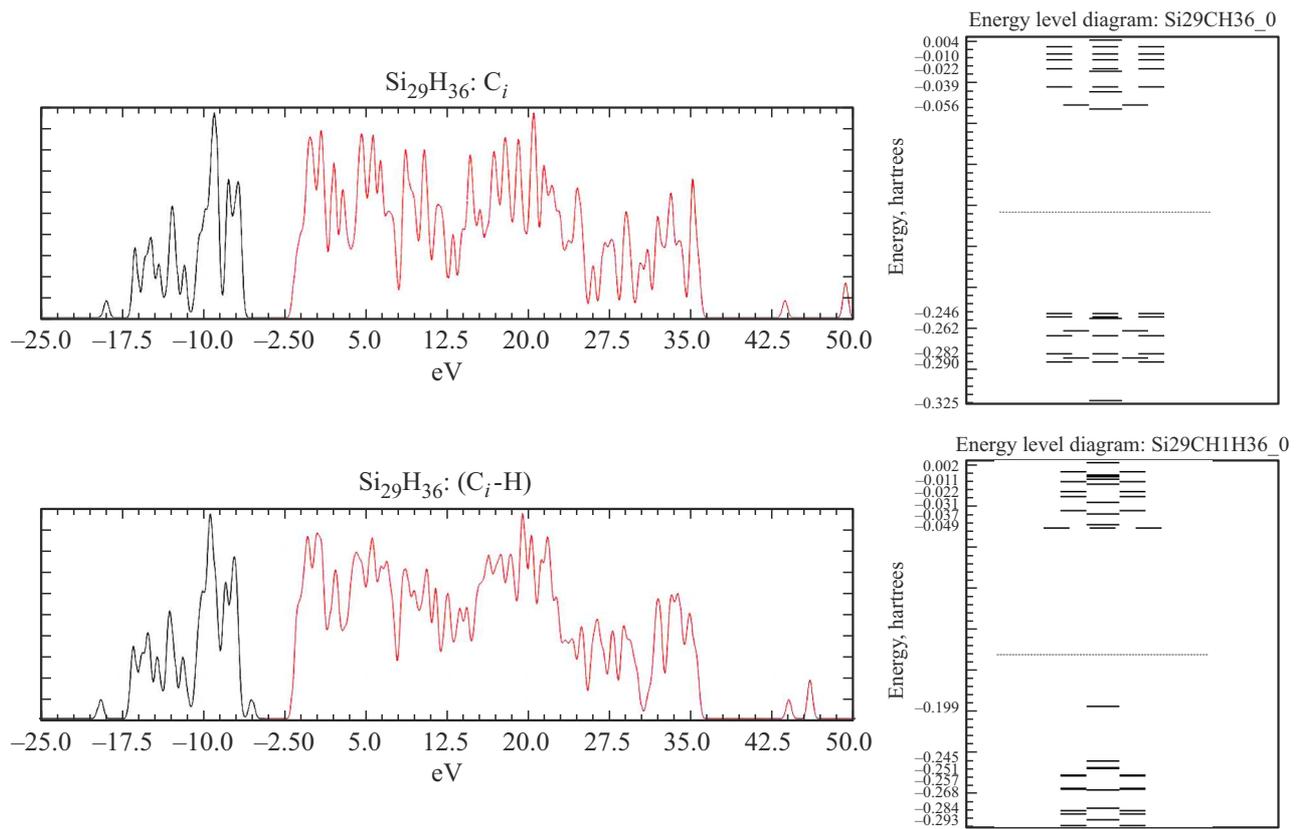
Si$_{29}$H$_{36}$: (C$_i$-H)

Figure 3. Formation of energy levels in the band gap in a Si$_{29}$H$_{36}$ cluster due to the introduction of impurity carbon and hydrogen atoms.

impurity carbon atom contributes to the emergence of a deep level in the band gap of a cluster, forming a defect H−C center (see the plot in Fig. 3). The second H atom may be restrained near the defect. Hydrogen forms strong bonds with an interstitial defect, where the H binding energy is −3.14 eV. The formed structural defect states with hydrogen migrate fast and react readily with other defects, suppressing their concentration. Electrical activity is abated in the presence of H atoms.

It follows from Table 2 that the binding energy of a carbon–hydrogen defect complex with a silicon cluster decreases in hydrogenated clusters. At the same time, positive and neutral charge states of a defect yield local levels deep within the band gap, while a negative state produces a shallow level above the valence band of a nanocluster.

Binding energies of a defect complex were calculated using the formula from [20,21] with the binding energy of atoms of a defect with interstitial carbon and hydrogen in a silicon cluster taken into account:

$$E_f = E(\mathrm{Si}_{n-1}X\mathrm{H}_i\mathrm{H}_m) - E(\mathrm{Si}_n\mathrm{H}_m) + \mu_{\mathrm{Si}} - \mu_X + l\mu_{\mathrm{H}}, \quad (7)$$

where E_f is the formation energy of a defect complex, $E(\mathrm{Si}_{n-1}X\mathrm{H}_l\mathrm{H}_m)$ is the total energy of a hydrogenated cluster with a defect, $E(\mathrm{Si}_n\mathrm{H}_m)$ is the total energy of a hydrogenated cluster without a defect, μ_{Si} is the total energy

of a single silicon atom in this cluster, μ_X is the total energy of a single carbon atom in this cluster, and μ_{H} is the total energy of a single hydrogen atom in this cluster (if two or more H atoms are introduced into the local environment of a carbon atom, factor l is used; i.e., l is the number of interstitial H atoms in the region around C_i).

The results of calculation of energy parameters of a C_i-H defect complex in a silicon nanocluster are listed in Table 2.

It follows from Table 2 that the C_i-H binding energy in a cluster depends only weakly on the charge state of H and is specified by the number of hydrogen atoms in a cluster. Hydrogenation of dangling bonds of a cluster results, on the one hand, in defect stabilization and, on the other hand,

Table 2. Energy parameters of a C_i-H defect complex in a silicon nanocluster

	Binding energy of a defect complex, eV	E_{LUMO}, eV	E_{HOMO}, eV	E_g, eV
Si$_{29}$: C$_i$H	12.34	−8.29	−8.19	0.10
Si$_{29}$: C$_i$H(+)	12.58	−8.04	−7.93	0.11
Si$_{29}$: C$_i$H(−)	12.15	−8.57	−8.47	0.10
Si$_{29}$H$_{24}$: C$_i$H	7.53	−8.67	−8.15	0.52
Si$_{29}$H$_{24}$: C$_i$H(+)	7.68	−8.06	−7.11	0.95
Si$_{29}$H$_{24}$: C$_i$H(−)	7.45	−9.31	−9.22	0.09

in weakening of bonds between an impurity C_i atoms with surrounding Si atoms.

4. Conclusion

The examination of structure and electronic states of silicon nanoclusters containing carbon atoms and interstitial hydrogen atoms revealed that impurity carbon atoms in an interstitial-site state form a bridge bond with two silicon atoms and are located at a hexagonal site at the center of the cell. A negatively charged carbon state strengthens the bond. A single impurity carbon atom produces shallow levels in the band gap of nano-silicon.

It was demonstrated that the presence of one hydrogen atom in the vicinity of C_i promotes the formation of a C_i-H-Si defect complex and reduces the defect binding energy in a $Si_{29}:C_i$ cluster.

It was also found that positive and neutral charge states of a defect yield local deep levels within the band gap of a nanocluster, while a negative state produces a shallow level.

The presence of hydrogen leads to neutralization of an electrically active state of a shallow level in a $Si_{29}:C_i$ cluster. The structural and energy state of a C atom in a C_i-H-Si defect complex depends on the number of hydrogen atoms.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] M.G. Mil'vidskii, V.V. Chaldyshev. Semiconductors, **32**, 457 (1998).
[2] K.L. Brower. Phys. Rev. B, **9**, 2607 (1974).
[3] G.D. Wotkins, K.L. Brower. Phys. Rev. Lett., **36**, 1329 (1976).
[4] A. Mattoni, F. Bernardini, L. Colombo. Phys. Rev. B, **66**, 195214 (1-6) (2002).
[5] D. Tsuchiya, K. Sueoka, H. Yamamoto. Phys. Status Solidi A, **216**, 1 (2019).
[6] A.Ya. Nashel'skii. *Proizvodstvo poluprovodnikovykh materialov* (M., Metallurgy, 1989) p. 272.
[7] V.I. Fistul'. *Atomy legiruyushchikh primesei v poluprovodnikakh* (M., Fizmatlit, 2004) (in Russian).
[8] Z.M. Khakimov, P.L. Tereshchuk, N.T. Sulaymonov, F.T. Umarova, M.T. Swihart. Phys. Rev. B, **72**, 115335 (2005); M.Yu. Tashmetov, A.B. Normurodov, N.T. Sulaymanov, Sh. Makhkamov, F.T. Umarova, A.V. Khugaev, Kh.M. Kholmedov. J. Nano-Electron. Phys., **10**, 0301 (1−6) (2018).
[9] Z.M. Khakimov. Comput. Phys. Commun., **147**, 733 (2002).
[10] K. Raghavachari, C.M. Rohlfing. Chem. Phys. Lett., **167**, 559 (1990); Run-Ning Zhao, Zi-Chen Lu, Rui Chenaand Ju-Guang Han. Phys. Chem. Chem. Phys., **21**, 25302 (2019).
[11] P. Deák, T. Frauenheim, M.R. Pederson (eds). *Computer Simulation of Materials at Atomic Level* (Berlin, 2000) Chap. 3; T. Frauenheim, G. Seifert, M. Elstner, Z. Hajnal, G. Jungnickel, D. Porezag, S. Suhai, R. Scholz. *A Self-Consistent Charge Density-Functional Based Tight-Binding Method for Predictive Materials Simulations in Physics, Chemistry and Biology.*
[12] Z.M. Khakimov. J. Phys.: Conf. Ser., **29**, 177 (2006).
[13] V.P. Markevich, B. Hourahine, R.C. Newman, R. Jones, Mats Kleverman, Lennart Lindström, L.I. Murin, M. Suezawa, S. Öberg, P.R. Briddon. // Publication in Lund University research portal /http://www.scientific.net/3-908450-83-7/. **221** (2), 1 (2003).
[14] M.V. Kovalenko, L. Manna, A. Cabot, Z. Hens, D.V. Talapin, C.R. Kagan, V.I. Klimov, A.L. Rogach, P. Reiss, D.J. Milliron, Ph. Guyot-Sionnest, G. Konstantatos, W.J. Parak, T. Hyeon, B.A. Korgel, Ch.B. Murray, W. Heiss. ACS Nano **9**, 1012 (2015).
[15] E. Van Lenthe, E.J. Baerends. J. Comp. Chem., **24**, 1142 (2003).
[16] A.K. Shiryaev. *Kvantovaya mekhanika i kvantovaya khimiya* (Samara, Samar. Gos. Tekh. Univ., 2014) (in Russian).
[17] L.V. Spivak, N.E. Shchepina. *Fiziko-khimicheskie osnovy protsessov mikro- i nanotekhnologii* (Perm, Permsk. Gos. Nats. Issled. Univ., 2018), Part 1 (in Russian).
[18] D.M. Fleetwood, S.T. Pantelides, R.D. Schrimpf. *Defects in Microelectronic Materials and Devices* (N.Y., Taylor & Francis Group, 2009) p. 737.
[19] Vl. Kolkovskya, R. Stübnerb, K. Gwozdzc, J. Weber. Physica B, **535**, 128 (2018).
[20] Z. Zhou, R.A. Friesner, L. Brus. J. Am. Chem. Soc., **125**, 15599 (2003).
[21] Sh. Makhamov, F.T. Umarova, A.B. Normurodov, N.T. Sulaymanov, O.B. Ismailova. Uzbek. Phys. J., **18**, 82 (2016).

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