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The First Principal Calculation of The Electronic Structure of The Ge Strained Layers and the Set of Ge Islands on (001) Si Film

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Electronic properties of the Ge strained layers (3 mono layers from 24 atoms on the cell) on (001) Si film (2 mono layers from 16 atoms on the cell) and the set of Ge pyramidal islands (3 mono layers from 7 atoms on the cell) on Si film are investigated by our computer program package based on the density functional theory and pseudopotential to obtain quantum – mechanical ground state electronic configuration. These atom systems are participants of the process of the conversion from the 2D epitaxial growth of the strained heterostructures to the 3D nano islands growth. As a result studies it was appeared significant space localization of the electronic density in the Ge islands as compared with the Ge continuous strained film. So the facts are as follows the trace of electronic density is still observed on the distance of 3,6 Å from the surface of the Ge film whereas this distance from the Ge islands top is only 2,4 Å. As for the electronic energy spectrum for the set of Ge islands on Si film the valence bands overlap and their top falls.

Key words: the Ge strained layers on (001) Si film; the set of Ge islands on (001) Si film; the first – principal calculation; the electronic structure.

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Introduction

One of the efficient directions of the shaping of the nanostructures are the using the self organized growing islands in process of the molecular beam epitaxy of the strained heterostructures in accordance with the Stranski – Krastanow mechanism. The physical essence of this shaping of the nanostructures is concluded in reduction of the strain energy when turning from the two-dimensional layer growing to the three-dimensional island growing. So, growing of the germanium film on silicon is accompanied the appearance elastic deformations which appear because of mismatch their lattice constants. These atom systems are participants of the process of the spontaneous conversion from the 2D layer epitaxial growth of the strained heterostructures to the 3D nanoislands growth. In large many cases in the literature data is considered mechanism of three-dimensional island nucleation and relaxation of strained two-dimensional layers in heteroepitaxy of germanium on silicon, which accompanies spontaneous island growth [1,2] while theoretical studies of electronic properties such structures are absent practically. Aims of our work are efficient investigation properties of noted above atomic systems by means of a first principles description of electronic structure. For this objective theory of functional of electron density and an ab initio norm-conserving pseudopotential within the framework

of algorithm of quantum-mechanical molecular dynamics were used.

I. Calculation method and results

Calculations for these atomic systems were performed within the local density approximation. The electron-ion interaction has been modeled by ab initio norm-conserving pseudopotential. The ground state electronic and atomic structures and its energy were obtained by “dynamical simulated annealing” (the Car-Parrinello method – the CP method) [3]. For the calculation the superlattice geometry was chosen. The translate symmetry was required for simplify mathematic expression. The atomic basis of the primitive tetragonal unit cell of the superlattice reflected features of the investigating system. It comprised from 8 atoms to 66 atoms of silicon and/or germanium depending on the investigating system. The calculation algorithm means using of atomic basis which certainly can to have inverse symmetry. The location of atoms simulated Si crystal (8 atoms in atomic basis), Ge crystal (8 atoms in atomic basis), Si(4 layers)/Ge(4 layers) heterostructures (Ge strained layers) (64 atoms in atomic basis), Si(2 layers)/Ge(6 layers) heterostructures (Ge strained layers) (64 atoms in atomic basis), Si(2 layers)/Ge(3 layers) film with free Ge (001) surface (Ge strained layers) (64 atoms in atomic basis) , the set of Ge pyramidal islands (3

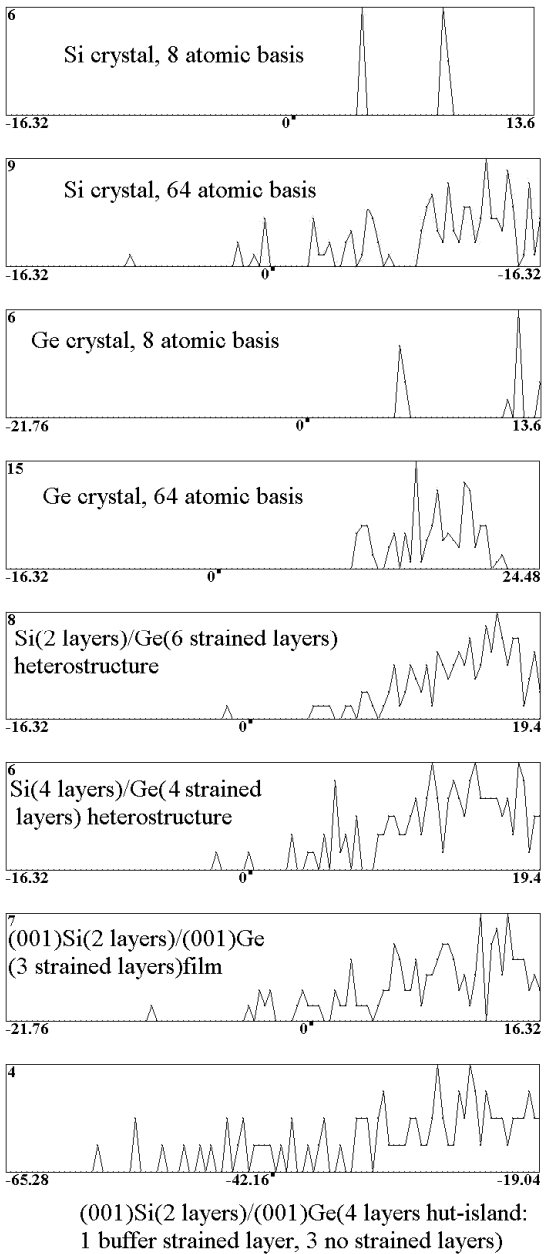


Fig. 1. Amount of electronic states, which account for valent and forbidden zone in Γ -point of Brillouin zone (energy is expressed in eV).

layers in “hut” - islands and 1 buffer strained layer) on Si (001) film (2 layers) (46 atoms in atomic basis) or the set of Ge pyramidal islands (3 layers in “hut” - islands on Si (001) film (2 layers) (30 atoms in atomic basis).

Using the author program code [4], the performances of the basic state of atomic systems for center of Brillouin zone have been received under on such variants of requirements of experiment: (1) number of plane waves in decomposition of the complete wave function of system has made from 20 to 160 plane waves on a atom depending on size of the atomic basis; value of fictitious mass for the orbitals dynamics – 300 atomic unities, a time step in algorithm of the molecular dynamics – 2 atomic unities, number of iterations of the self-coordination – 20; starting conditions for electronic

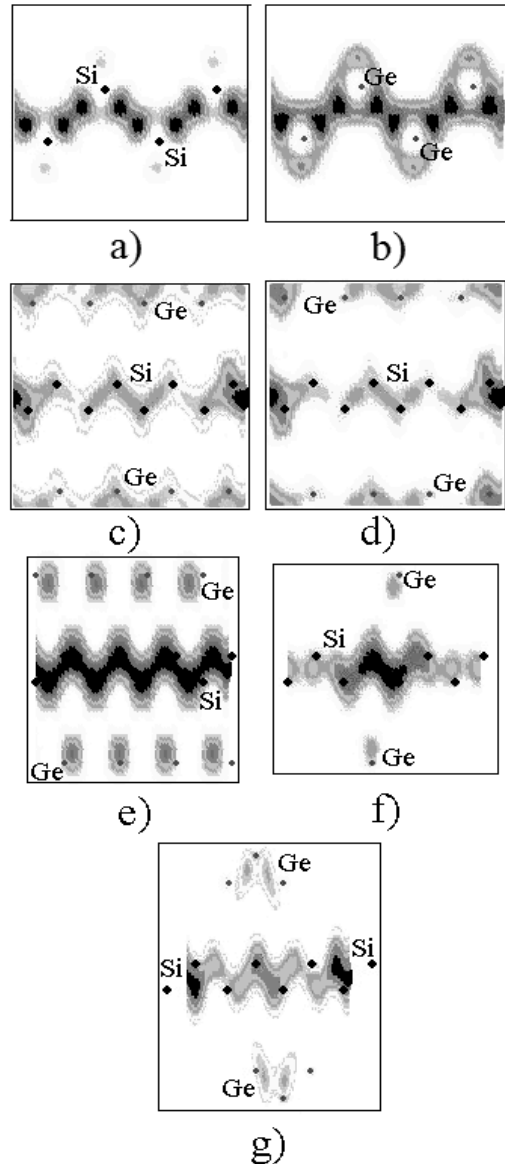


Fig.2. The (110) section of the space valence electron density distribution: (a) for bulk silicon; (b) for bulk germanium; (c) for Si (4 layers)/Ge (4 layers) heterostructures (Ge strained layers); (d) for Si (2 layers)/Ge (6 layers) heterostructures (Ge strained layers); (e) for Si (2 layers)/Ge (3 layers) film with free Ge (001) surface (Ge strained layers); (f) for the set of Ge pyramidal islands (3 layers in “hut” – islands) on Si (001) film (2 layers); (g) for the set of Ge pyramidal islands (3 layers in “hut” - islands and 1 buffer strained layer) on Si (001) film (2 layers).

orbitals were defined by random values of coefficients in decomposition of the lowest states and zero velocities of their change; interaction of valence electrons with an ion of a atom core was calculated with the help of Hartwigsen, Goedecker, Hutter ionic pseudopotential from first principles which took into account contributions s-, p-, d- orbitals [5]; (2) under other identical requirements, starting conditions for electronic orbitals were defined Hamiltonian matrix

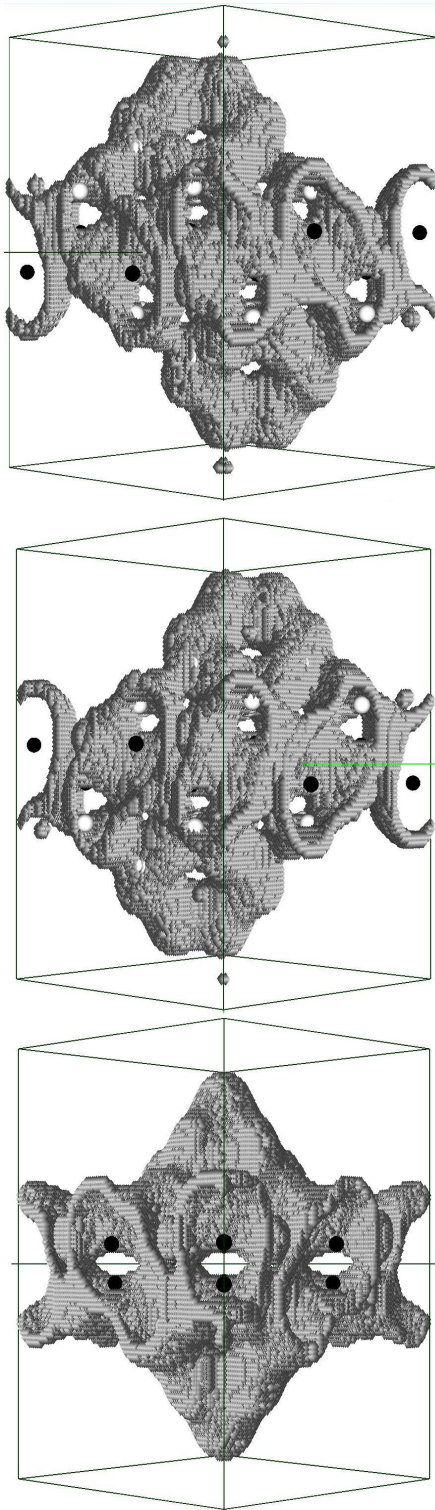


Fig.3. The space valence electron density distribution for the atomic composite of the set of Ge pyramidal islands (3 layers in “hut” - islands and 1 buffer strained layer) on Si (001) film (2 layers) (density from 0.1 to 0.2 from of the maximum value). It is seen what disappear the area to electronic density responsible for interaction, when increase the parameter of the lattice.

diagonalization, which has consisted from functional of a kinetic energy and the Bachelet – Hamann - Schluter ionic pseudopotential which took into account contributions s-, p-, d- orbitals [6] and have been screened by the dielectric function in Thomas-Fermi approximation.

For observation of transformation of electron density at change of dimensionality and atomic composition of investigated objects on fig. 2, 3 sections of a spatial distribution of electron density are given. Brought results were received without optimization of the coordinates of atoms that is to say coordinates had importance according to stipulated above atomic basis. The optimized coordinates got by method of molecular dynamics, small differed from source.

Inspection of the maps of valence electron density distributions allowed to definite the principal properties of the electronic structure of this atomic composite. As a result studies it was appeared significant space localization of the electronic density in the Ge islands as compared with the Ge continuous strained film (Fig.2. e, f, g). So the facts are as follows the trace of electronic density is still observed on the distance of 3,6 Å from the surface of the Ge film whereas this distance from the Ge islands top is only 2,4 Å. On drawing Fig.3 it is seen what disappear the area to electronic density responsible for interaction, when increase the parameter of the lattice (that is to say increases vacuum gap between films in superlattice).

On drawing fig. 1 it are shown electronic states, which account for valent and forbidden zone in Γ - point of Brillouin zone. So, for the set of Ge islands on Si film it is characteristic of essential change to location of the allowed electronic states. As follows it appeared much separated states, herewith, the whole set of the states fell on energy.

Conclusions

Electronic properties of the Ge strained layers on (001) Si film and the set of Ge pyramidal islands on Si film are investigated by our computer program package based on the density functional theory and pseudopotential. It was appeared significant space localization of the electronic density in the Ge islands as compared with the Ge continuous strained film. For the set of Ge islands on Si film it is characteristic of essential change to location of the allowed electronic states, as follows it appeared much separated states.

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Розрахунок із перших принципів електронної структури напружених шарів Ge та масиву островків Ge на плівці (001) Si

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Досліджені електронні властивості напружених шарів Ge (3 моно шари із 24 атомів на елементарну комірку) на плівці (001) Si (2 моно шари із 16 атомів на елементарну комірку) та масив пірамідальних островків Ge (3 моно шари із 7 атомів на елементарну комірку) на плівці (001) Si авторським пакетом комп'ютерних програм, що ґрунтуються на теорії функціоналу електронної густини та псевдопотенціалу і дозволяють отримати основний стан електронної підсистеми. Ці атомні системи являються учасниками процесу переходу від 2D епітаксимального росту механічно напружених гетероструктур до 3D росту нанострівок. В результаті досліджень було встановлено суттєву просторову локалізацію зарядової густини в Ge острівках у порівнянні з неперервними напруженими плівками Ge. Вона проявлялася в тому, що залишки електронної густини ще спостерігалися на відстані 3,6 Å від поверхні плівки Ge, тоді як ця відстань від вершин Ge острівків була тільки 2,4 Å. Стосовно енергетичного спектра електронів у масиві островків Ge на плівці Si, спостерігається перекриття валентних зон та зниження їх вершин.