Structure and Formation Energies of Ge Atoms Surface Complexes on the Substrate Si(001)(4×2)

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Nowadays there is no complete understanding of the physical chemistry of the formation of germanium nanodots Ge/Si, especially with regard to the initial stages of Ge atoms and Ge_2 dimers adsorption on the verge of Si(001), due to the lack of reliable data studied and mismatch between there. In experimental studies, the usually structure and properties of Ge islands are determined, and the initial stages of their formation remain unaddressed. In this case, methods of quantum chemistry are useful, which allow us to study nanostructures at atomic level, in particular to clarify the main features of the primary stages of the interaction of germanium atoms with a silicon substrate.

Calculations were performed using density functional theory with the base set 6-31G ** and hybrid exchange-correlation functional B3LYP using a software module GAMESS.

These experimental studies and quantum chemical calculations allowed to offer four different configurations Ge_2 dimers on the surface of silicon dimers on the verge of Si(001)(4×2) (Fig. 1.)

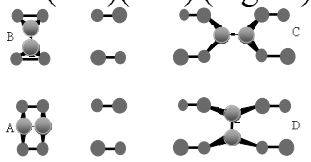
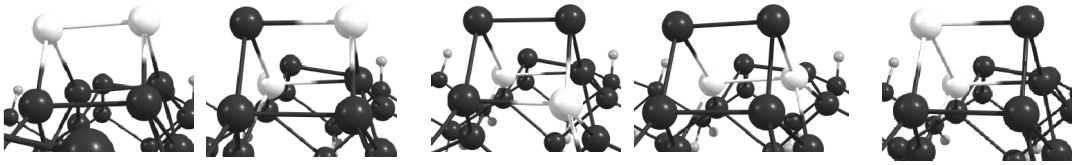


Fig. 1. Schematic representation of the structure of possible adsorption complexes of Ge_2 on the verge of the reconstructed Si(001)(4×2) surface.

In addition to the formation of clean germanium surface structures, penetration of possible the atoms in to the first substrate layer or more in the deeper layers.

Closest in is energy to the configuration A (A0 in Fig. 2) was A1 configuration that differed from A0 by shift of one *down*-atom in the bulk and by moving in to its place of the silicon atom of the substrate. The energy of this process is 80 meV. The energy difference between the configurations A0 and A1-A4 (see Fig. 2) is quite small, suggesting their possible reciprocal transformation at room temperature, without taking into account the activation barrier of the transitions between them.



A (0) A1 (80 meV) A2 (120 meV) A3 (220 meV) A4 (220 meV)

Fig. 2. The configuration of Ge–Ge dimer (A0) and configurations formed from it by the interchange of Ge atoms and Si atoms on substrate Si(001)(4×2).