Atomistic modeling of step formation and step bunching at the Ge(105) surface

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Abstract

We investigate possible step geometries on the rebonded-step reconstructed Ge(105) surface. We focus our attention on steps oriented along the [010] direction, which have been shown to play a key role in the pyramid-to-dome transition during Ge growth on Si(001). Using molecular dynamics simulations based on the Tersoff potential, we evaluate the step formation energy for several alternative structures. The step-bunching process is also analyzed, showing that one monolayer-high steps are likely to group into multistepped structures. Our results provide support for very recent experiments and modeling on the pyramid-to-dome transition in Ge/Si(001).
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1. Introduction

It is well known that the deposition of Ge onto Si(001) leads to the nucleation of three-dimensional nanometric islands, which first appear as pyramids bounded by {105} facets [1–4]. After increasing their volume up to a critical size, a very interesting morphological evolution is observed. The island base becomes more rounded and steeper facets appear, leading to the so-called dome geometry [2,3]. Very recent, high-resolution scanning tunneling microscope (STM) images provided a detailed microscopic description of the pyramid-to-dome transition [5]. The transition starts at a critical size, at the apex of the (105) pyramid, which grows faster than the rest of the island. As a consequence, a set of (105) steps dividing the upper and lower region are imaged by STM. Further evolution produces a pronounced bunching of such steps, facilitating the creation of the steeper facets, which are typical of the dome geometry. The situation is sketched in Fig. 1 for the initial

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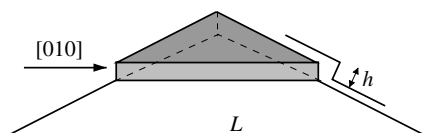*E-mail address:* silvia.cereda@unimib.it (S. Cereda).

Fig. 1. Schematic representation of a Ge pyramid grown on Si(001) in the metastable stepped state detected by STM images in Ref. [5]. For the sake of simplicity, a single step, of height h, is traced, along the [010] direction. L represents the length of the island base.

configuration where a single (105) step appears. In Ref. [5] a simple model is shown to well reproduce the above described experimental evidence. At the top of the pyramid the average lattice parameter is well known to be close to the bulk Ge one, while at the base it approaches the Si value. As a consequence, next-layer nucleation is energetically favoured at the pyramid top (see also the discussion in Ref. [6]). Small pyramids, however, never display a stepped structure in the STM images, since the cost of forming a step (scaling linearly with the island's basis length, L) exceeds the gain provided by placing more Ge atoms towards the pyramid top (scaling as L^2). On the contrary, above the critical volume the number of steps accumulated towards the pyramid apex increases with L. The model in Ref. [5] contained a single fitting parameter, i.e. the step formation energy Γ, while the other energy contributions were estimated by using the Tersoff potential [7]. A good agreement between the model and the experiments (appearance of stepped pyramids for $L \sim 50$ nm) was obtained for Γ values of ~ 12 meV/Å.

In the present paper, we shall provide an independent estimate of Γ based on atomistic simulations. Upon considering various possible step configurations we shall characterize the lowest-energy step configuration. Furthermore, we shall investigate the energetics of the step bunching process on the (105) surface, with the aim of providing further theoretical support to the model of Ref. [5].

2. Steps at the {105} pyramid facets

The (105) surface, as-cut, is a typical vicinal surface, displaying arrays of (001) terraces separated by steps (see Fig. 2). In this work we do
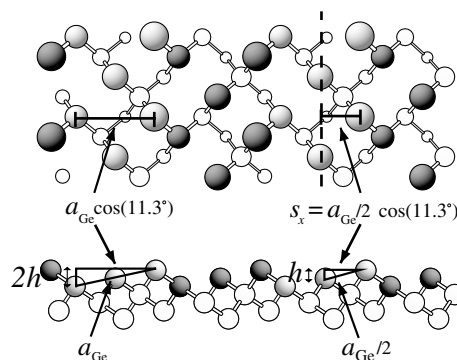

Fig. 2. Top view of the (105) surface in the as-cut configuration. Atoms on different (001) terraces are here in different gray shade. s_x is used to indicate the shifted stacking between two adjacent (105) layers separated in height by $h \sim 0.55$ Å.

not investigate such steps, but steps delimiting adjacent (105) terraces of different height. In fact, the (001) steps are removed by a peculiar rebonded-step (RS) reconstruction [8–11], which takes place at the {105} Ge-pyramid facets on Si(001) [12], turning them into flatter surfaces [11]. While a detailed description of the RS geometry can be found in Refs. [8–12], here we briefly recall that such a reconstruction is characterized by the formation of U-shaped structures (Us), illustrated in Fig. 3, closely resembling the typical atomic arrangement found at S_B steps on (001) surfaces (see Fig. 3 of Ref. [11]). The Us are open on one side (the tails of the Us in the following) and closed by a dimer on the other one (head of the Us). The atomic density in any Ge(105) layer is of ~ 0.025 atoms/Å^2, with only ~ 0.55 Å (h) separating adjacent (105) planes [11] (see Fig. 2 in which the as-cut geometry is shown). The comparison of these values with the Ge(001) ones (atomic density of 0.068 atoms/Å^2 and interplane distance of ~ 1.4 Å) shows that the (105) planes are very open, with high stacking density.

For simplicity here we should focus only on steps oriented along the pyramid base, e.g. the [010] direction sketched in Fig. 1, mostly relevant in changing the facet steepness [5]. Let us imagine now to select a terrace bounded by two parallel steps along the [010] direction on the (105)RS surface, as large as the surface periodicity. It is clearly seen in Fig. 3 (where two hypothetical step posi-