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Schwoebel barrires as the reason for 3D-island formation during heteroepitaxy

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Abstract. Self-assembled 3D-islands formation during heteroepitaxial growth was investigated by Monte Carlo simulation. Shwoebel barriers for explanation of 3D growth kinetic were suggested. Island size equalization during growth process was observed. Necessity of atomic flux from island edge to the upper layers for 3D island formation was demonstrated.

Heteroepitaxial growth have been utilized for the generation of strongly strained coherent 3D islands, named quantum dots (QDs) [1, 2]. The elastic energy of the initially planar strained layer increases during heteroepitaxial growth. The system can lower its free energy by atom transitions from the island edge to the upper layer as that leads to decrease of contact area between substrate and new layer [1, 3–6]. Kinetic of such process could be described taking into consideration diffusion peculiarities when an atom crosses island edges. Additional energy barriers for atoms crossing monoatomic step (Schwoebel barriers) are suggested to be responsible for QD formation [7, 8]. Kinetic problems of epitaxial growth with Shwoebel barriers were considered theoretically in [9]. Increase of nucleation rate of islands in the second monolayer was associated in [10] with asymmetry of Schwoebel barriers in SiGe system.

Introduction of additional energy barriers E_{st} for atom hops over monoatomic steps in the model enable us to investigate Schwoebel barriers influence on surface relief formation during epitaxy [11]. Diffusion hop probability to cross the step is changed by the factor $P = exp(-E_{st}/kT)$ as compared with diffusion hops at the same atomic level. Factor P_{up} changes probability of atom hops to the upper layers, and P_{down} — to the lower ones. Phase diagram in coordinates $P_{\text{up}} - P_{\text{down}}$ is presented in Fig. 1(a). Shaded area — Stransky-Krastanov growth mode – separates layer-by-layer regime (2D) from 3D-island growth

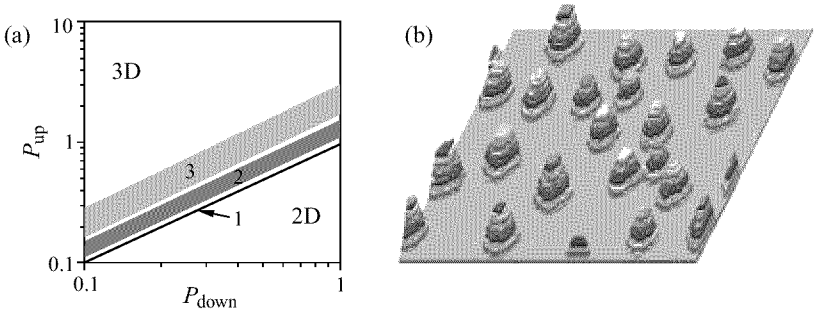

Fig. 1. (a) Phase diagram indicating conditions for 3D islands formation, shaded area — Stransky–Krastanov growth mode, 1 — line $P_{\text{up}} = P_{\text{down}}$, 2 — $\lambda = 40$ a.s., 3 — $\lambda = 20$ a.s.; (b) simulated surface after 1.5 ML deposition, $\lambda = 20$ a.s., $\chi = 10$.

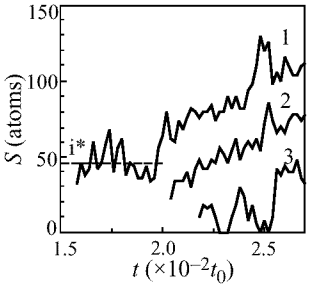

Fig. 2. Number of atoms in three successive atomic layers of 3D island formed at $\lambda = 40$ a.s. versus time for $\chi = 2$ (figure at the curve corresponds to atomic layer number), i^* — critical (2D) nucleus size (CNS).

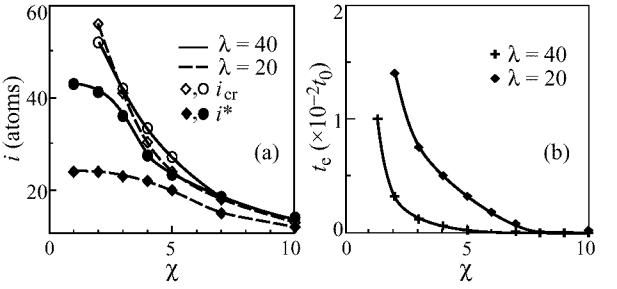

Fig. 3. (a) CNS dependence on χ; (b) expectation time t_e for appearance of the nucleus of the second monolaeyr on 2D islands versus χ.

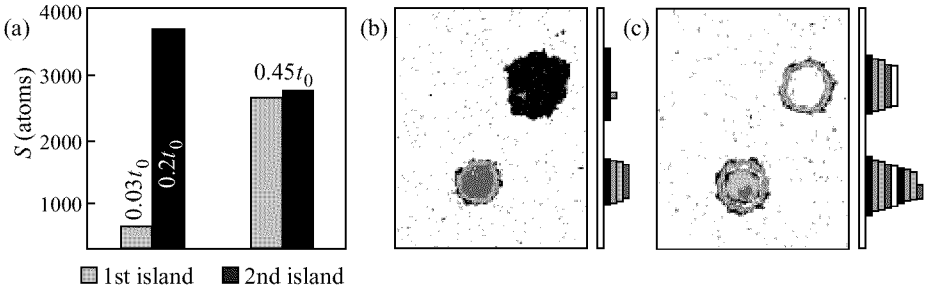

Fig. 4. Islands self-organization during growth process, $\lambda = 40$ a.s.: (a) histogram of size redistribution of two islands with time, left columns correspond to the moments of the second layer nucleus creation on 2D islands; top view of model surface (200 × 250 a.s.) after deposition 0.2 ML (b) and 0.45 ML (c), to the right of each surface — its profile (b-c).

mode. Shaded area is parallel to the line $P_{up} = P_{down}$ which is to say that the change-over from 2D to 3D mode (2D $\longrightarrow$ 3D) is determined only by the parameter $\chi = P_{up}/P_{down}$ and not by the absolute values P_{up}, P_{down}. Notice that for 3D island formation without wetting layer condition $\chi > 1$ is necessary. Increasing of migration adatom length $\lambda(D/V)$, (D — surface diffusion coefficient, V — deposition rate) leads to parallel shift of transition 2D $\longrightarrow$ 3D to the lower values P_{up}, under condition $\chi > 1$. Figure 1(b) represents the model surface with 3D islands.

Number of atoms in three successive atomic layers of 3D island formed on (100) surface at $\lambda = 40$ atomic sites (a.s.) versus time is shown in Fig. 2. Fig. 2 demonstrates stable 2D-island formation till 3D island growth starts. Size of this 2D island fluctuates about average value i^*, that is equal to critical nucleus size (CNS). Large CNS corresponds to active exchange between islands and equilibrium adatom gas due to small binding energy between neighboring atoms. For equilibrium conditions following relationship was obtained $i^* \sim (D/V)^{1/5}$ that means slight increase of i^* with λ increase. As one can see in Fig. 2 CNS decreases in each next atomic layer.

The critical size of island i_{cr} when nucleation of new layer starts is of interest. Dependence $i_{cr}(\chi)$ was investigated. Dependencies i^* and i_{cr} on χ for two λ are presented in

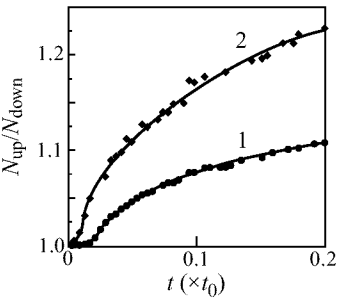

Fig. 5. N_{up}/N_{down} (ratio of absolute number of hops to the upper layers to hops to the lower layers) dependence on time; $\lambda = 40$ a.s., 1 — $\chi = 2$, 2 — $\chi = 10$.

Fig. 3(a). As χ increases these sizes decrease approaching 1 for $\chi \longrightarrow \infty$. From some χ, $i^* = i_{cr}$, that means 3D nucleation from the initial phase of growth. Expectation time t_e for appearance of the nucleus of the second monolaeyr on 2D islands versus χ is represented in Fig. 3(b). This dependence is exponential one: $t_e(\chi) = \tau_0 \cdot \exp(-\alpha \cdot \chi)$. For $\lambda = 40$ a.s. — $\tau_0 = 0.017 \cdot t_0$, $\alpha = 0.8$, and for $\lambda = 20$ a.s. — $\tau_0 = 0.035 \cdot t_0$, $\alpha = 0.5$, where t_0 – time necessary of one monolayer deposition.

3D islands without wetting layer demonstrate rather sharp size distribution. That is due not only to the most synchronous 2D island nucleation in the first atomic layer. Lateral size equalization when 3D growth process starts (case of large size fluctuation of initial 2D-islands) could be seen in Fig. 4. Figure 5 demonstrate increase with time of hops up to hops down ratio N_{up}/N_{down}. Such N_{up}/N_{down} variation is due to decrease of atoms capable to attach into descending island boundary because of their attachment to the island of upper layer.

Acknowledgements

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