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Simulation of pores sealing during homoepitaxy on Si(111) surface

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Abstract. Simulation of homoepitaxy process on porous Si(111) using 3D Monte Carlo model was carried out to give estimation of necessary dose for complete pores overgrowth of different sizes, porosity and various deposition flux intensities for given temperature.

Porous silicon (PS) is one of the most promising materials for Si-based emitting devices that can be useful in integrated optoelectronics [1, 2]. Recently an approach to fabricate a compliant substrate for growing high-quality heteroepitaxial layers was proposed [3]. A double layer of PS obtained from heavily doped p-type Si was used as the substrate. A low-porosity top layer and a bottom layer with high porosity act as a mechanical damper between heterostructure and a massive support and allow to grow GeSi film without misfit and threading dislocation. The same idea was used when growing GaAs layer on thin Si layer over porous Si substrate [4]. Usually there are only circumstantial evidences that porous substrate is overgrown [5, 6]. Number of deposited layers necessary for complete pores healing is of great importance for highquality heteroepytaxial growth on porous substrates.

3D model of epitaxy on the surfaces of diamond like crystals [7] was applied for analysis of epitaxy on (111) porous silicon surfaces. Our lattice model can take into account atoms from surface region up to hundred atomic layers in the depth. One monolayer could contains up to 10^5 atoms. The main event in the model is diffusion hop, with atom hopping to the empty lattice site in the first, second or third coordination spheres. Adsorption process is considered to be independent on diffusion. Voids and vacancies in the bulk, multilevel steps and deep pores on the surface are possible. The abandonment of solid-on-solid (SOS) principle permits atoms movement along the walls of steps and pores.

Simulation of homoepitaxy process on porous Si(111) was carried out giving estimation of necessary dose for complete pores overgrowth of different sizes, porosity and deposition rate. Simulations were carried out in the following ranges of substrate parameters: porosity $13 \leq P_s \leq 64\%$, pores diameter: 3.5–14 nm and rather wide ranges of deposition rate, according to experimental works [3, 5, 6]. In the model deposition rate is introduced through the universal parameter $n_{dif} \sim D/V$, where D is diffusion coefficient and V-deposition rate. Simulation results of epitaxial growth on porous surface with 100×100 atomic sites (a.s.) at $T = 1073$ K [5, 6] for different surface porosity, pores sizes and deposition rate $V = 0.004-40$ nm/min) are presented in Fig. 1–4. For given temperature one can estimate deposition rate according to the formulae $V = \nu \cdot \exp(-E_d/kT)/n_{dif}$, where E_d is activation energy for surface diffusion (eV), V is deposition rate (bilayer per second, BL/s), ν is vibration frequency (1/s), k is Boltzmann's constant, T is substrate temperature (K). Taking $\nu = 10^{13}\ s^{-1}$, $E_d = 1.75$ eV [7], $T = 1073$ K for $n_{dif} = 10^5$ 1/BL one obtains $V = 0.6$ BL/s.

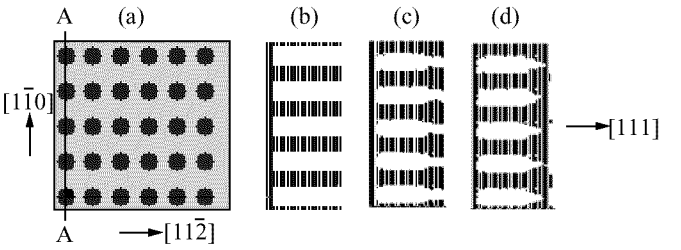

Fig. 1. Homoepitaxy simulation on porous Si(111) surface at $T = 1073$ K for $n_{\text{dif}} = 10$ (high deposition rate). Pores diameter is 10 atomic sites, height is 20 BL, surface porosity $P_s = 26$ %. (a) initial surface top view; (b) initial cross-section AA along [011] direction; (c) cross-section AA after 1.5 BL deposition; (d) cross-section AA after 3.1 BL deposition.

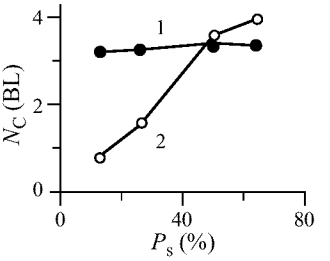

Fig. 2. Dependence of minimum number of deposited bilayers necessary for complete pores overgrowth N_c on porosity P_s for small pores for high and low deposition rates: pores diameter 10 a.s. $T = 1073$ K, (1) — $n_{\text{dif}} = 10$ ($V = 6000$ BL/s), (2) — $n_{\text{dif}} = 10^5$ ($V = 0.6$ BL/s).

Plan view and cross-section along [011] direction for the surface with small pores and surface porosity $P_s = 26\%$ before and after deposition with high deposition rate could be seen in Fig. 1. For these conditions it was necessary 3.1 BL of silicon to be pores completely overgrown. Figure 2 demonstrates dependence of minimum number of deposited bilayers necessary for complete pores healing (N_c) on surface porosity P_s for low and very high deposition rates and small pores. For high deposition rate N_c is independent of porosity and for low V N_c increases with P_s. This dependence is clear: for high deposition rate atoms reaching pores are gathered only from small region around each pore limited by migration length. For porosity less than 65% and deposition rates under examination migration length is less than average distance between pores. For low deposition rate all adatoms on the surface are involved in healing process, so the higher porosity the less numbers of atoms are left on the surface (portion of atoms falls to the bottom of the pores). Figure 3 demonstrates dependence of N_c on n_{dif} for three different pores sizes. For large pores strong dependence of flux intensity is observed. Large number of deposited layers N_c is necessary for complete pores sealing for high deposition rate ($N_c > 40$ BL) while for low flux N_c is rather small and has only weak dependence on pores diameter. In the latter case N_c is determined by deposited dose rather than diffusion, so dose limited regime takes place. Figure 4 illustrates N_c dependence on porosity for different pores sizes (Fig. 4(a)) and on pores size for different deposition rates (Fig. 4(b)). N_c independence of porosity for high deposition rate is evident from curves Fig. 4(a) and was discussed above. Linear dependence of N_c on pore diameter for low deposition rates is clear from curves 2, 3 while curve 1 ($n_{\text{dif}} = 10$, corresponds to high deposition rate) demonstrates superlinear dependence. Cross-sections along [011] direction before (a) and after deposition (b-c) on porous Si(111) surface with

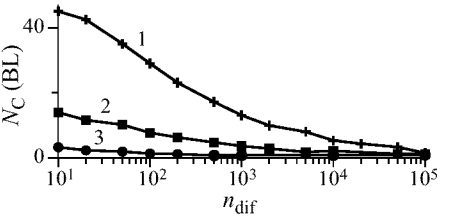

Fig. 3. Dependence of N_c on n_{dif} for different sizes of pores. $T = 1073$ K, porosity $P_s = 26\%$, pores diameter: (1) — 40 a.s., (2) — 20 a.s., (3) — 10 a.s.

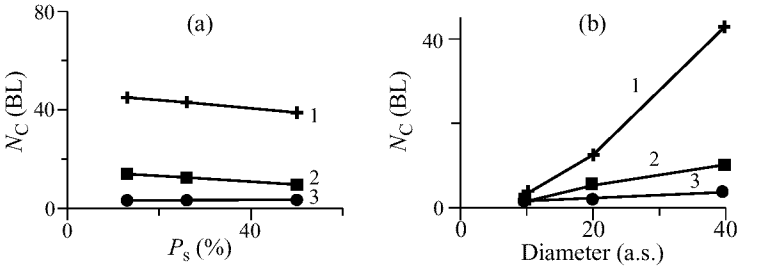

Fig. 4. $T = 1073$ K (a) Dependence of N_c on porosity P_s for high deposition rate: ($n_{dif} = 10$) for different sizes of pores: pores diameter: (1) — 40 a.s., (2) — 20 a.s., (3) — 10 a.s.; (b) Dependence of N_c on pores size for porosity $P_s = 26\%$ and different growth rate: (1) — $n_{dif} = 10$, (2) — $n_{dif} = 10^3$, (3) — $n_{dif} = 10^5$.

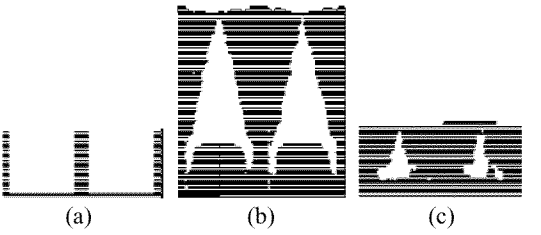

Fig. 5. Homoepitaxy simulation on porous Si(111) surface at $T = 1073$ K for high and low deposition rates, surface porosity $P_s = 50\%$, pores diameter 40 a.s., height 20 BL. (a) initial cross-section along [011] direction; (b) cross-section after 37.7 BL deposition for high deposition rate ($n_{dif} = 10$); (c) cross-section after 9.6 BL deposition for low deposition rate $n_{dif} = 10^5$.

surface porosity $P_s = 50\%$ and large pores are presented in Fig. 5. The differences in sealing process are evident from these figures. For high deposition rate (Fig. 5(b)) overgrown pores have cone shape with convex up bottom and N_c is found to be rather large. In this case migration length is small and adatoms create islands as between pores on the surface as on pores bottom. Atom flux in our simulation is perpendicular to the surface. Overhanging walls arising during growth process are beneficial for whiskers formation along pores walls near the bottom. Quite different situation one has for low deposition rate (Fig. 5(c)). At the initial stage of growth pores shape keeps nearly invariable, only diameter of each pore is decreasing due to larger migration length of adatoms mooving along pores walls. Final sizes of buried pores in the latter case are noticeable smaller.

Acknowledgements

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References

[1] B. Surma, A. Wnuk, A. Misiuk, A. Brzozovski, M. Pawlowska, M. Franz, J. Jun, M. Rozental and E. Nossarewska-Orlowska, *Cryst. Res. Technol.* **34**, 689 (1999).

[2] T. J. Rinke, R. B. Bergmann and J. H. Werner, *Appl. Phys. A* **68**, 705 (1999).

[3] S. I. Romanov, V. I. Mashanov, L. V. Sokolov, A. Gutakovski and O. P. Pchelyakov, *Appl. Phys. Lett.* **75**, 4118 (1999).

[4] Y. Hayashi, Y. Agata, T. Soga, T. Jimbo, M. Umeno, N. Sato and T. Yonehara, *Jpn. J. Appl. Phys.* **37, P2, N11B**, 1354 (1998).

[5] T. Ito, T. Yasumatsu and A. Hiraki, *Appl. Surf. Sci.* **44**, 97 (1990).

[6] Y. Yasumatsu, T. Ito, H. Nishizawa and A. Hiraki, *Appl. Surf. Sci.* **48/49**, 414 (1991).

[7] A. V. Zverev, I. G. Neizvestny, N. L. Shwartz and Z. Sh. Yanovitskaya, *Izv. RAS (Russian)* **63**, 356 (2000).