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Molecular beam epitaxy (MBE) is well established as one of the premier techniques in nanostructure fabrication. Especially, MBE growth of GaAs on a cleaved (110) surface (cleaved-edge overgrowth method) is becoming of increasing importance as a fabrication method for novel semiconductor nanostructures with high quality. The overgrowth on a cleaved (110) surface requires, however, a low substrate temperature range and a very high As₄-vapor overpressure for GaAs and overgrown film has rough surfaces with $4\sim$ 5-ML-high pits and islands.

We have recently found that rough as-grown (110) surface turns to an atomically smooth surface if we perform growth-interrupt in-situ annealing at 600 °C for 10 min. This annealing method has enabled us to realize quantum wires and wells with unprecedentedly high quality. For example, a quantum well after annealing shows an atomic smoothness over the entire 80 μ m x 0.38 mm area which corresponds on a more human scale to a flatness perfection over a 3.8 km region.

On the other hand, surface regions with average thickness deviated from integer-ML forms characteristic stepedges shapes such as isolated 1-ML-deep pits and 2-to-3-ML-high islands. We performed statistical analysis on the size and shape distribution of the 1-ML-deep pits. Figure 1 shows a model for the formation of atomic stepedges, which is based on the stability of atomic sites. Our model, namely Ga atom migration occurs from two-bond sites to three-bond sites having higher stability, well explained the driving force to form an atomically smooth surface and characteristic atomic step-edges [1].

We also performed the first-principles calculation on the migration barrier energy for Ga and As adatoms on a GaAs (110) surface [2]. These results shows far smaller barrier energies than those on another GaAs surfaces, which enable adatoms to migrate in a very long length and explain the formation of a very wide atomically smooth (110) surface as stated above.

Figure 2 (a) and (b) show the calculated potential surfaces for the Ga and As adatoms on the GaAs (110) surface. Note the difference between the two contour maps (a) and (b). Ga adatoms migrates along the [110] direction in 1-D way as migration barrier energy surface has low-energy trenches along this direction. On the other hand, the energy surface of the As adatoms is 2-D. It should be noted that for both Ga and As adatoms, the stable near As of the topmost layer are very stable, while those near Ga are unstable. This fact explains the asymmetric shapes of 1 ML deep pits shown in Fig. 1 (a). The lower stability of two-bond step-edges (A-D and B-C) compared with three-bond step-edges (A-B and C-D) causes atom migration from two- to three-bond stepedges and makes the pit elongated along [110]. Both Ga



FIG. 1: (a) Top and side views of the atomic arrangement model of a 1-ML-deep pit observed on the annealed (110) surface. This model has the Ga-terminated three-bond stepedge (A-B), the As-terminated three-bond step-edge (C-D), and the two-bond step-edges (A-D and B-C). (b) Atomic step kinetics of the surface evolution during annealing. Proposed schematic drawings of the evolution for the island and pit structures from an assumed square initial shape are obtained by considering detachment and incorporation of Ga atoms from the ($\overline{110}$) or ($1\overline{10}$) edges to the (001) and ($00\overline{1}$) edges at the surface during annealing.



FIG. 2: Contour map of migration barrier energy for (a) Ga adatom and (b) As adatom on a GaAs (110) surface with the surface atomic configuration. The dotted and solid circles correspond to As and Ga, respectively.

and As adatoms feel repulsion from the Ga-terminated step-edge (A-B), while they feel attraction from the Asterminated step-edge (C-D). Thus, adatom density becomes high near the C-D edge. Therefore, for both Ga and As adatoms, the corner sites C and D are the most stable sites for incorporation into the step edge. The repetition of such incorporation processes makes the fish-like shape of the pit.

Authors

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