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Semiconductor Surface Studied by TEM: Si (001) 2x1 Reconstructed Surface and Heterogrowth of Ge

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Atomic structures of the reconstructed surfaces of Si(001)2x1 and heteroepitaxy of Ge on Si(001) seen by UHV electron microscopy are shown. Roles of bilayer and monolayer steps for heteroepitaxial growth on the reconstructed surface are clarified.

1. INTRODUCTION

UHV electron microscopes are used in transmission(TEM-TED) and reflection(REM-RHEED) modes of observation. They have "insitu" facilities for surface cleaning. heating, deposition and gas reaction $^{1,2)}$. A high resolution UHV electron microscope developed recently, having a point-to-point resolution of 0.21nm and vacuum of 10⁻⁸Pa level. is used for revealing surface structures on atomic scale¹⁾. In this report, bilayer-monolayer geometry of the Si(001)2x1 surfaces and heteroepitaxial growth of Ge on them are shown to demonstrate the importance of microscope study on surface and interface problems.

Roles of steps on Si(001)2x1 surfaces are particularly noticed in the heteroepitaxial growth of $GaAs/Si(001)^{3-5}$. $GaAs/GaAs(001)^{6}$ and $GaAs/Ge(001)^{7}$. It is considered that single GaAs films grow without anti-phase domain boundaries on surfaces with bilayer-high steps³⁾, while single domain GaAs films were found to grow even on surfaces with monolayer-high steps^{4,5)}. In case of the heteroepitaxy of Ge on Si(001), related to strained-layer superlattice, it is not clarified why higher density of defects are introduced to the interface between Ge and Si substrate than that expected from the lattice mismatch of Si and Ge, $4\%^{8)}$, and why three dimensional islands grow after layer-by-layer growth up to 4 monolayers(ML)⁹⁾. Most of these observations were done by RHEED, but scarcely done are microscope studies^{10,11}.

2. Si(001)2x1 SURFACE

The doubling of surface periodicity in the 2x1 reconstructed surface is due to dimer formation. For specimens with a concave (convex) surface, the geometry of bilayer and monolayer steps is given in figs. 1 and 2^{11} . The bilayer steps tend to be parallel to dimer direction of the 2x1 reconstructed surfaces¹²⁾, being separated by about 2 - 7 nm on surfaces of $7 - 2^0$ off toward [110] (or [110] direction). They become unstable, however, on surfaces inclined toward [100] (or [010] direction), so that they split into monolayer steps (see fig. 2). Stability of the monolayer and

bilayer steps, rebonded and unrebonded types of atomic geometries is discussed by $Chadi^{13}$ in favor of the geometry in fig. 1.



Fig. 1 Geometry of bilayer and monolayer steps on a concave Si(001)2x1 surface. Bilayer steps are shown by chain lines and monolayer steps are, by dotted lines. Dimer directions are indicated. Displacement vectors of 2x1 unit cells across bilayer step, R+ or R-, are shown. Bilayer steps are stable on surfaces of the off-angles, 2-7°, toward directions within 20° about the [110] direction.

3. GROWTH OF Ge ON Si(001)2x1

Growth process of Ge on Si(001) surface at 650° C was observed by REM images of the specular reflection as seen in fig. 3. The images are foreshortened in the beam direction of the [110] (vertical direction in the figures). In an image of clean Si(001) surface before the deposition of Ge, fig.3(a), darkly and brightly contrasted areas are domains of 2x1 (dimer are parallel to the [110]) and 1x2 (dimers are vertical to the [110], respectively, being separated by monolayer steps(0.136nm). These steps are classified into two types, A and B, according to whether the direction of the dimer of the upper terrace is vertical or parallel to the [110] step as shown in (a). By deposition of Ge, type A steps moved towards the lower sides of the step (from right to left), while type B steps almost stayed at their initial positions as seen in (b), (c) and (d), where the deposited amounts are 0.7, 1.1and 1.4ML, respectively. (1 ML corresponds to Ge atoms of $6.78 \times 10^{14} / \text{cm}^2$.) At 1.4 ML the entire surface was nearly converted to the 2x1 (dark area), and several structure Ge islands nucleated on the first Ge layer. In the RHEED pattern, superlattice spots from the 2x1 domain, which are seen on the 0th order Laue zone in fig.4(a) of clean Si(001) surface, are seen in fig.4(b) of the surface In addition, the 8th order of fig.3(d). superlattice reflections appear in fig.4(b), which are similar to those observed in case of quenched clean Si(001) surface¹⁴⁾. Tn case that the terraces were wide enough, monolayer islands of Ge nucleate on them, and out of phase boundaries were formed when they touched with each other or when they touched to steps. Such out of phase boundaries were noticed to work as preferential nucleation sites for the other Ge islands, which results in the surface roughness. Details of these observations will be reported separately¹⁵⁾.



Fig. 2 REM image of Si(001)2x1 surface. Wavy zig-zag lines are image of surface monolayer steps, so that dimer direction changes 90^{0} at every steps alternately, as indicated. Note widths of terraces between steps $A_1^{-A_4}$ change alternately as fig. 1.



Fig. 3 REM images ([$\overline{110}$] incidence) of a growth process of Ge on Si(001) surface at 650° C. Type A steps move as the deposit amount of Ge increases, while type B steps almost stay at their initial positions.



Fig. 4 RHEED patterns, (a) clean Si(001) surface(fig.3(a)), (b) 1.4ML of Ge deposited surface(fig.3(d)).

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