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Monte Carlo Analysis of Microstructures in Ordered III-V Semiconductor Alloys : Attempt of Simulation for the triple period (TP-A) structure

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Recently, TP-A ordered phase was found in $Al_{0.48}In_{0.52}As$ grown on (001) InP substrate by Gomyo et al. In the present paper, we propose a new crystal growth model which can consider the effects of a complex surface reconstruction on ordering. Monte Carlo simulation of TP-A ordering was carried out under two different conditions ; for the cases of a perfect 2x3 surface reconstruction and of the reconstruction with an anti-phase boundary. The simulation resulted that plate like domains of ordered phase were formed in the former case, and microdomains of ordered phase in the latter case. The latter result was found to reproduce the experimental result well.

1. INTRODUCTION

Various types of ordered phases have been reported in III-V semiconductor alloys [1-3] . The most commonly observed type is CuPt. Understanding the ordering mechanism is important for device processing, since the ordering affects the material properties such as the band gap energy and electron mobility.

Recently, a new type of ordered phase was found in $Al_{0.48}In_{0.52}As$ grown on (001) InP substrate by Gomyo et al. [4]. The period along <111>A direction in the ordered structure is three times as long as that of the (111) spacing, and the atomic sequence of group-III is .../XYZ/XYZ/XYZ/... along the <111>A directions ,where $X=Al_xIn_{1-x}$, $Y=Al_yIn_{1-y}$, $Z=Al_zIn_{1-z}$. The new phase is called "triple-period (TP-A)" ordered phase. The ordered phase is thought to be formed on the 2x3 surface reconstruction.

In the present paper, we will report some results obtained by Monte Carlo simulations of TP-A ordering.

2. MODEL AND SIMULATION METHODS

We previously proposed a crystal growth model [5], which is applicable to epitaxial growth, and simulated the CuPt($L1_1$)-type ordering using the Monte Carlo method [6-10]. We have developed a new crystal growth model in order to take into account effects of complex surface reconstruction on ordered phase. It is assumed here that the surface reconstruction during growth is (2x3) (see Fig. 1). Atomic layers of $(A_{0.48}B_{0.52})^{III}$ and C^{V} are accumulated epitaxially on an exactly oriented (001) substrate. The composition ratio is based on the experimental data. When a plane of Group-III atoms is on the top surface during growth, A and B atoms exchange their positions to lower the configuration energy. The configuration of 60x60 atoms is frozen-in when they are covered with the next surface plane. An epilayer of 60 planes is grown by repeating the above process.

The details of simulation method are as follows. The position of an *fcc* sublattice of Group-III elements ($\vec{r}$) is denoted by a vector,

$$\vec{r} = n\vec{a} + m\vec{b} + l\vec{c} \qquad (1)$$

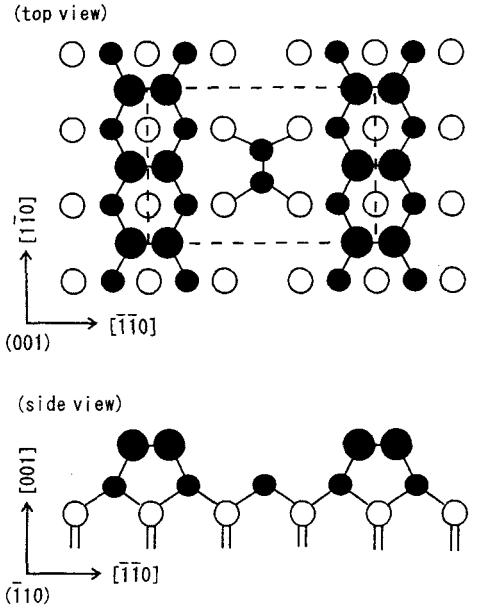

Fig. 1 A possible model for the 2x3 surface reconstruction. The open and filled circles indicate the group-III atoms and group-V atoms, respectively.

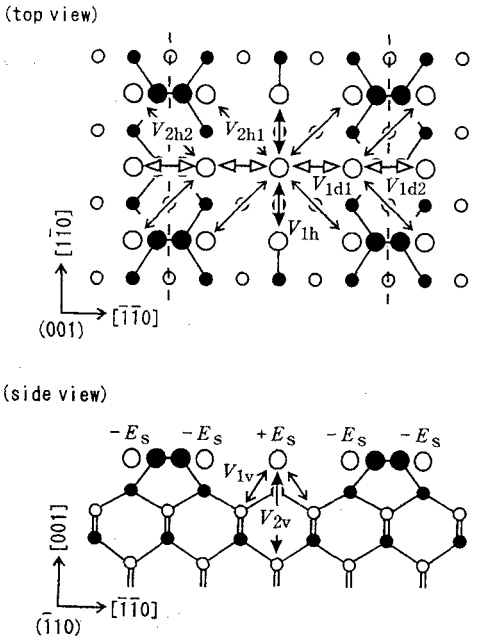

Fig. 2 The pairwise interaction parameters near the crystal surface.

where $\vec{a},\vec{b}$ and $\vec{c}$ are the primitive translation vectors of the *fcc* sublattice, defined as

$$\vec{a}=\tfrac{1}{2}[1\bar{1}0],\ \vec{b}=\tfrac{1}{2}[110],\ \vec{c}=\tfrac{1}{2}[10\bar{1}] \quad (2)$$

for convenience. Here, *n,m* and *l* are integers. The origin of the coordinate is placed at an *fcc* sublattice of Group-III elements in the top surface. Thus the surface lattice points are characterized by l=0. The configurational term Ec in the internal energy for the surface plane of A and B atoms is assumed to be given by

$$\begin{aligned} Ec = &-\tfrac{1}{2}\sum_{\vec{r}_1(l=0)}\sum_{\vec{r}_2(l=0)} V(\vec{r}_2-\vec{r}_1)\gamma(\vec{r}_1)\gamma(\vec{r}_2) \\ &-\sum_{\vec{r}_1(l=0)}\sum_{\vec{r}_2(l>0)} V(\vec{r}_2-\vec{r}_1)\gamma(\vec{r}_1)\gamma(\vec{r}_2) \\ &-\sum_{\vec{r}_1(l=0)} Es(\vec{r}_1)\gamma(\vec{r}_1), \end{aligned} \quad (3)$$

with the pairwise interaction parameters $V(\vec{r}_2-\vec{r}_1)$, the site-occupation operators $\gamma(\vec{r})=\pm 1$ and the site-correlation energy $Es(\vec{r})$. The system prefers unlike atom pairs if V is negative, or like-pairs if it is positive. A-atom tends to take the site $\vec{r}_1$ if Es is positive, and B-atom tends to if it is negative. Figure 2 shows the pairwise interaction parameters considered in the crystal surface. Here, open and filled circles denote atomic sites for III and V elements, respectively. V1d1 and V2h1 indicate the pairwise interaction parameters when there is not a Group-V atom between the pair of Group-III atoms, and V1d2 and V2h2 indicate the ones when there are Group-V atoms between the pair of Group-III atoms. The detail of definition of other pairwise interaction parameters are indicated in Ref. 6 and 8. Group-III atoms pair in the top surface plane exchange their positions with the probability [11]

$$W=\frac{\exp(-\Delta Ec/k_BT)}{1+\exp(-\Delta Ec/k_BT)}. \quad (4)$$

Here, ΔEc shows the difference in configuration energy between after and before exchange of the

atom positions, k_B is the Boltzmann constant, and T is the growth temperature. We adopt the relative values of parameters which well reproduce the TP-A ordering ; $V1h > 0$, $V1d1 = -|V1h|$, $V1d2 = |V1h|$, $V1v = |V1h|$, $V2h1 = -0.5|V1h|$, $V2h2 = 0.5|V1h|$, $V2v = -0.3|V1h|$, $Es>0$ and $T=|V1h|/k_B$.

3. RESULTS AND DISCUSSION

Figures 3(a) and (b) show $(\bar{1}10)$ projection of atomic configuration and $(\bar{1}10)$Fourier power spectrum obtained by the simulation of the (001) epitaxial growth, respectively. In Fig. 3(a), one can see plate-like domains of the TP-A ordered phase. In the Fourier power spectrum of this atomic configuration (Fig. 3(b)), superlattice sp arise at $h\pm\frac{1}{3}, k\pm\frac{1}{3}, l\pm\frac{1}{3}$ and $h\mp\frac{1}{3}, k\mp\frac{1}{3}, l\pm$ which indicate the TP-A ordering. Streaks ly parallel to the growth direction are caused by outward of the system. According to the TI observations carried out by Gomyo et al. [4 microdomains of TP-A ordered phase w formed in the crystal, being different from results of the simulation. We tried simulating the case where APBs (anti-phase boundari exists in the 2x3 surface reconstruction in orde reproduce the feature of microstructure. Ea surface layer has APBs which are perpendicu to the three times period direction of the surf reconstruction. The positions of APB in ea surface layer is random. Figures 4(a) and show the $(\bar{1}10)$ projection of atomic configurati and the $(\bar{1}10)$Fourier power spectrum obtained

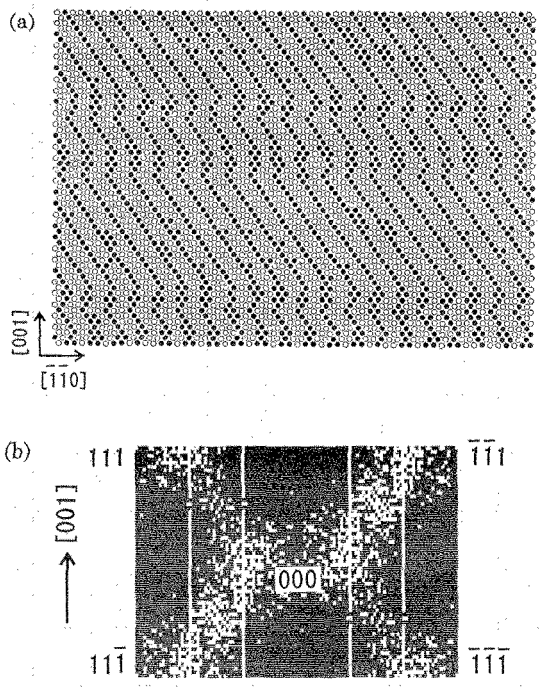

Fig. 3 (a) $(\bar{1}10)$ projection of atomic configuration. The filled and open circles indicate the atomic column contain A-atom-rich and B-atom-rich, respectively. (b) $(\bar{1}10)$ Fourier power spectrum.

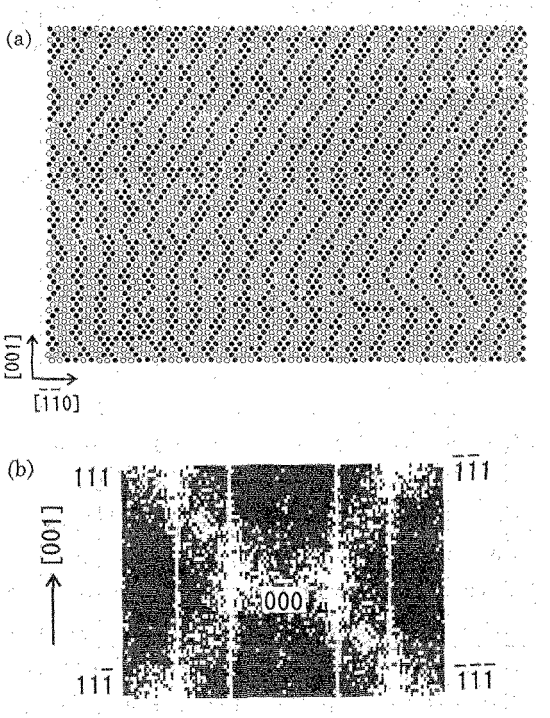

Fig. 4 (a) $(\bar{1}10)$ projection of aton configuration. (b) $(\bar{1}10)$ Fourier power spectrun

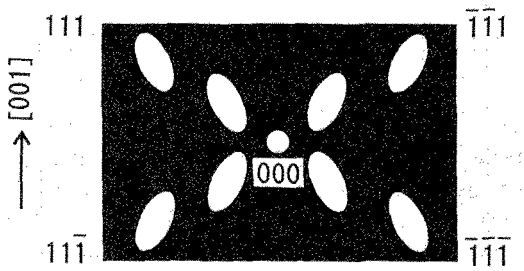

Fig. 5 The feature of $(\bar{1}10)$ electron diffraction pattern reported by Gomyo et al. The streaks are tilted toward growth direction.

In Fig. 4(a), we can find that the feature of microdomain structure observed by TEM is well reproduced. The ordered phase is thought to be prevented by the APBs from horizontal development and then become to microdomains embedded in the matrix. Figure 5 illustrates schematically the feature of $(\bar{1}10)$ electron diffraction pattern reported by Gomyo et al. The elliptic superlattice spots are tilted toward the growth direction. Fig. 4(b) reproduces this feature well. From these simulation results, we conclude that the microdomain structure is formed on an "imperfect surface reconstruction" which contains APBs. If the surface reconstruction during growth is perfect, the plate-like domains will be formed.

4. SUMMARY

It is thought that the TP-A ordered phase is formed on the 2x3 surface reconstruction. We develop a new crystal growth model which is able to take into account effects of surface reconstruction on ordered phase. We carried out the Monte Carlo simulations of the TP-A ordering using this model. In the case of the 2x3 surface reconstruction with APBs, microdomains of the ordered phase were formed. The result reproduces the experimental result well. Our calculations predict that plate-like domains are formed if the surface reconstruction is perfect without APB.

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