Diffuse scattering in partially ordered III-V semiconductor alloys

Manabu Ishimaru
Department of Materials Science and Engineering, Faculty of Engineering, Kyushu University 36, Fukuoka, Fukuoka 812-81, Japan

Syo Matsumura
Department of Nuclear Engineering, Faculty of Engineering, Kyushu University 36, Fukuoka, Fukuoka 812-81, Japan

Noriyuki Kuwano and Kensuke Oki
Department of Materials Science and Technology, Graduate School of Engineering Sciences, Kyushu University 39, Kasuga, Fukuoka 816, Japan

(Received 17 March 1995)

Features of diffuse scatterings in III-V semiconductor alloys grown on a (001) substrate have been investigated by Monte Carlo simulation, on the basis of a simple kinetic Ising model we proposed previously. Atomic arrangements and their Fourier power spectra were compared with previous experimental results reported by other researchers. An epilayer includes numerous (001) plane faults and platelike CuPt($L1_1$)-type ordered phases perpendicular to the growth direction. They give rise to the streaks along the [001] direction in an electron diffraction pattern. Our simulated result shows that the existence of like-atom clusters among the ordered domains causes the diffuse streaks drawn toward the fundamental lattice spots of a zinc-blende structure. With the progress of ordering, the wavy streaks become straightlike in shape and the position of their intensity maximum shifts from the $-(\frac{1}{2}-\delta)$, $\frac{1}{2}-\delta,0$ ($\delta>0$) to the $\frac{\bar{1}}{2}\frac{1}{2}\frac{1}{2}$ in the reciprocal lattice space. The results obtained here have explained quite well some characteristic features of the CuPt ordering in epilayers revealed by experiments. We also discussed the ordering process during the epitaxial growth by using Warren-Cowley parameters.

I. INTRODUCTION

It is well known that the atomic arrangement of III-V semiconductor alloys grown on a substrate depends on the method of sample preparation. The specimens grown by liquid-phase epitaxy possess a phase separated structure,[1-5] and this result is consistent with the phase diagrams for III-V semiconductor alloys in the *bulk* state which own miscibility gaps.[6-8] On the other hand, some ordered structures appear in the thin films obtained by vapor-phase epitaxy.[9] Their formation conflicts with the phase diagrams reported previously and raises an interesting problem in terms of thermodynamics. In addition, the appearance of ordered phases affects the band structure of the systems[10-13] and material properties such as the electron mobility. Therefore, the ordering mechanism in the epitaxial layers has been investigated by both experimental[14-19] and theoretical researches.[20-23] In the present study, we pay special attention to CuPt($L1_1$)-type ordering during the (001) epitaxial growth.

Previous transmission electron microscope observations[10,15-19] have found that a characteristic diffuse scattering appears in the short-range-ordered state of the III-V alloys. The streaks along the growth direction that pass through the $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ and the equivalent positions in the reciprocal-lattice space slant to the fundamental lattice spot of a zinc-blende structure. The shape of the diffuse scatterings and their intensity maximum position change with the development of ordering. That is, the curvature of the wavy streaks becomes small, and straight-shaped streaks appear in the well-developed epilayer.[15,16] In the epilayers obtained by low-growth temperatures or large deposition rates, the streaks have the maximum intensity around the fundamental lattice spots, $-(\frac{1}{2}-\delta),\frac{1}{2}-\delta,0$ ($\delta>0$). On the other hand, the position moves to the $\frac{\bar{1}}{2}\frac{1}{2}\frac{1}{2}$ indicating the presence of the CuPt-ordered phase in the case of high temperatures or small rates.[15,16,19] Why does the streak become wavy in the early stage of ordering and their shape and intensity maximum position change as a function of growth rate or temperature? This problem was relatively little explored, except for Otsuka's report.[24]

We have previously proposed a simple kinetic Ising model for the phase stability of atom configurations in epitaxial layers,[25] and carried out Monte Carlo simulation based on the proposed model.[26-28] Our model succeeded in explaining the CuPt-type-ordered microstructure in an epilayer deposited on an "off-angle" substrate[27] and reproducing features of electron diffraction patterns for off-stoichiometric III-V alloys.[28] The results suggest that the model is quite useful in discussing the ordering mechanism and the phase state in the III-V epilayers. In the present study, we apply our model to the layer-by-layer growth on an exact (001)-oriented substrate in order to clarify the relationship between the electron diffraction pattern and the microstructure in partially ordered III-V semiconductor alloys.

II. MODEL AND SIMULATION PROCEDURE

We now consider an epilayer of a semiconductor alloy of $(A_{0.5}B_{0.5})^{III}C^{V}$, which is growing via the layer-by-layer stacking on a substrate with an exact (001) orientation. Figure 1 shows pairwise atomic interactions for an atom on the (001) surface of a zinc-blende structure. Here, open and closed circles denote atomic sites for III and V elements, respectively. Atoms of A and B elements on the surface layer are assumed to interact with their first- and second-nearest-neighbor (1NN and 2NN) atoms in the fcc sublattice, and the internal energy of the system is given by the total sum of these interactions. The system prefers unlike-atom pairs (i.e., A-B) if the pairwise interaction parameter is negative, or like-atom pairs (i.e., A-A or B-B) if positive. The parameters are set so that unlike- and like-atom chains tend to be formed along the $[1\bar{1}0]$ and [110] directions, respectively, being coincident with the actual alloys.[15,17] The interaction parameters are set to be $V_{1h}<0, V_{1h}'=|V_{1h}|, V_{2h}=-0.5|V_{1h}|$ and $V_{2v}=-0.3|V_{1h}|$. The values for V_{1v} are given in the figure captions. Growth temperature is $T=|V_{1h}|/k_B$, where k_B is the Boltzmann constant. The subscripts h and v mean the (001) intraplane and interplane interactions, respectively. V_{1h} is of the 1NN pair which a C atom directly links, and V_{1h}' is of the 1NN one without the linkage, as indicated in Fig. 1(a).

In the present simulation, the (001) surface is given as a 64×64 grid with periodic-boundary conditions. A and B atoms are at first distributed randomly on the surface. Then, the positions of surface atoms are exchanged with each other over a given time interval following to Kawasaki dynamics.[29] The time interval for one-layer-stacking $\Delta\tau$ is measured in units of Monte Carlo step (MCS); one MCS in the present system corresponds to 4096 (64×64) attempts to exchange the atoms. The configuration of atoms thus obtained is considered to be frozen-in after being covered with the next surface plane, since the diffusion mobility of atoms is, in general, negligibly small within *bulk* III-V alloys. An epilayer with 64 planes of $(A_{0.5}B_{0.5})^{III}$ in thickness is grown by repeating the above procedure 64 times. Fourier power spectra of the resultant atomic arrangements are obtained for comparison with the actual electron diffraction patterns. Warren-Cowley short-range-order parameters,[30]

$$\alpha(r)=1-P_{BA}(r)/x\ ,$$

are also evaluated. Here, $P_{BA}(r)$ is the conditional probability of finding a B atom at a distance r from an A atom, and $x\,(=0.5)$ is the atomic fraction of B.

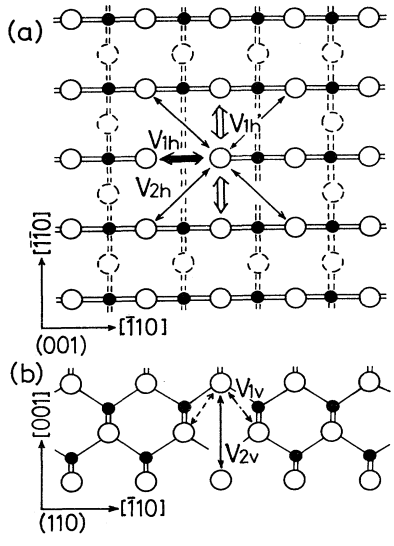

FIG. 1. Kinds of atomic pairs in fcc sublattices and their interactions for an atom on a (001) surface of a zinc-blende structure. (a) (001) and (b) (110) views. Open and closed circles indicate atomic sites for III and V elements, respectively. The double lines denote the covalent bonds.

III. RESULTS AND DISCUSSION

A. The appearance of wavy diffuse streaks

Figure 2 shows (110) Fourier power spectra of the atomic arrangements obtained by the layer-by-layer stacking. The 1NN interaction of the (001) interplane, V_{1v}, was set to be (a) negative, (b) zero, and (c) positive. Besides the fundamental lattice spots due to a zinc-blende structure, diffuse scatterings that pass through the $\frac{\bar{1}}{2}\frac{1}{2}\frac{1}{2}$ and the equivalent positions exist in the (110) spectra. On the other hand, it was confirmed that no extra reflections appear in the $(1\bar{1}0)$ patterns (not shown). That is, the epilayer contains only the $(1\bar{1}1)$ and $(\bar{1}11)$ variants termed $CuPt_B$ type. This variant selection originates from the fact that the four $\langle 111\rangle$ directions of the zinc-blende structure ($F\bar{4}3m$) that are symmetry equivalent in the *bulk* state are divided into two groups according to the bonding of atoms on {001} *surfaces*. As clearly seen, the curvature of streaks depends sensitively on the sign of V_{1v}. The streaks are drawn toward the fundamental lattice spots when V_{1v} is positive (c). In contrast, Figs. 2(a) and 2(b) have straight streaks and curved ones moving away from the fundamental points, respectively. The curvature of the wavy diffuse streaks in Fig. 2(c) is observed actually in the diffraction patterns reported previously,[10,15,16,19] showing that the value of V_{1v} should be positive in the III-V semiconductor alloys.

Figure 3 demonstrates Warren-Cowley parameters as a function of V_{1v}. The degree of order in (001) intraplanes and interplanes is distinguished, because the [001] direction which is parallel to the growth direction is not equivalent to the [100] and [010] directions in the case of the epitaxial growth. Here, the atom pairs are composed of like atoms if the parameter is positive and unlike atoms if it is negative. If a perfect CuPt-ordered phase is formed, the values of the even neighboring atoms become 1 or -1 and the values of the odd ones become 0. The degree of order of the (001) interplanes for Fig. 3(b) is larger than that for (a) and (c), suggesting that the finite value of V_{1v} disturbs the ordering. Actually, the formation of a secondary phase was confirmed from the analysis of atomic arrangements, as shown below. Note that the Warren-Cowley parameter of the 1NN interplane correlation $\alpha(1)$, which is indicated by the arrows, depends on the value of V_{1v}. The values of $\alpha(1)$ in (a),

(b), and (c) are negative, zero, and positive, respectively. This indicates that the epilayer for $V_{1v} > 0$ has a tendency to form like-atom pairs. In order to clarify the behavior of the $\alpha(1)$ depending on the sign of V_{1v}, we examined the atomic arrangements.

Cross-sectional views of the atom configurations which give Figs. 2(a) and 2(c) are shown in Figs. 4(a) and 4(b), respectively. The ordered structures with a double periodicity along the $[1\bar{1}1]$ or $[\bar{1}11]$ direction are formed in both diagrams, showing the appearance of two $CuPt_B$ variants. Besides the ordered domains, many antiphase boundaries and twin boundaries occur perpendicular to the growth direction. It is clearly seen that the streak along the growth direction in the (110) spectra is attributed to the (001) plane faults. Note in Fig. 4(a) that alternate stacking of A and B atoms along the [001] direction, or CuAu-I ($L1_0$)-type short-range ordering, is locally observed, while small like-atom clusters are dispersed in Fig. 4(b). The appearance of such structures consists with the behavior of $\alpha(1)$ in Fig. 3. From the calculation of configurational energy per one atom in the top surface, it was obvious that the CuAu-I structure and cluster are metastable phases in the case of $V_{1v} < 0$ and $V_{1v} > 0$, respectively. In summary, the positive V_{1v} interactions form such dispersed small like-atom clusters, and the additional tendency of clustering in 1NN atoms causes the wavy displacement of the streaks toward the fundamental reciprocal-lattice points.

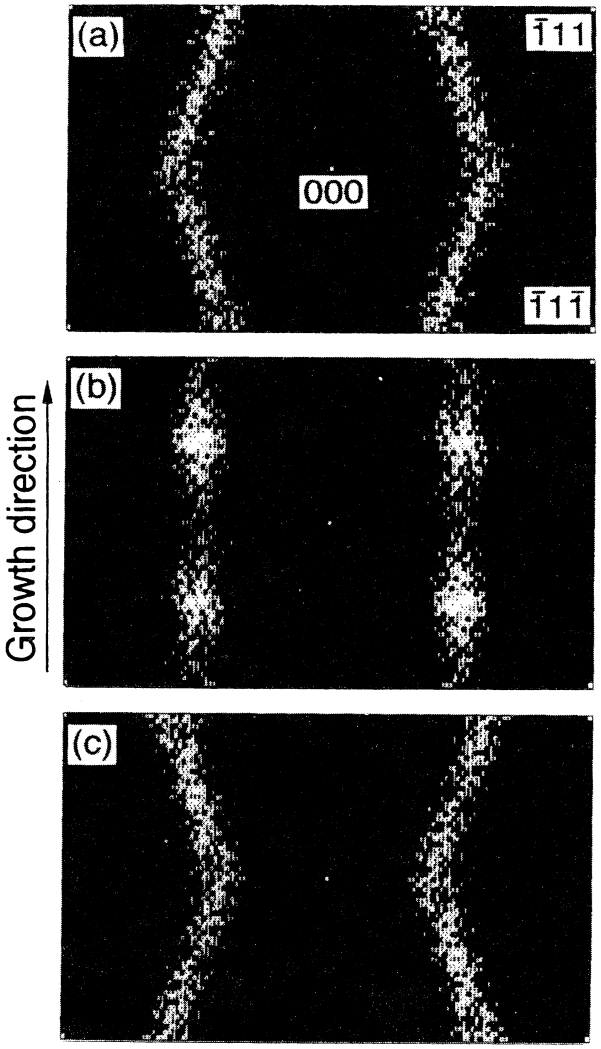

FIG. 2. (110) Fourier power spectra of the atom configurations in epilayers as a function of V_{1v}, which is for the interactions with 1NN atoms on the underlying plane. V_{1v} is equal to (a) $-|V_{1h}|(<0)$, (b) 0, and (c) $|V_{1h}|$ (>0), and the stacking time interval $\Delta\tau=20$ MCS. Diffuse streaks passing through the $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ and the equivalent positions appear along the growth direction, and their curvature depends on the sign of V_{1v}. The shape of streaks in (c) are in good agreement with that in the actual diffraction patterns reported previously.

B. Change of diffuse streak due to evolution of CuPt-type order

Figure 5 displays (110) Fourier power spectra as a function of the stacking time interval $\Delta\tau$. The increase in

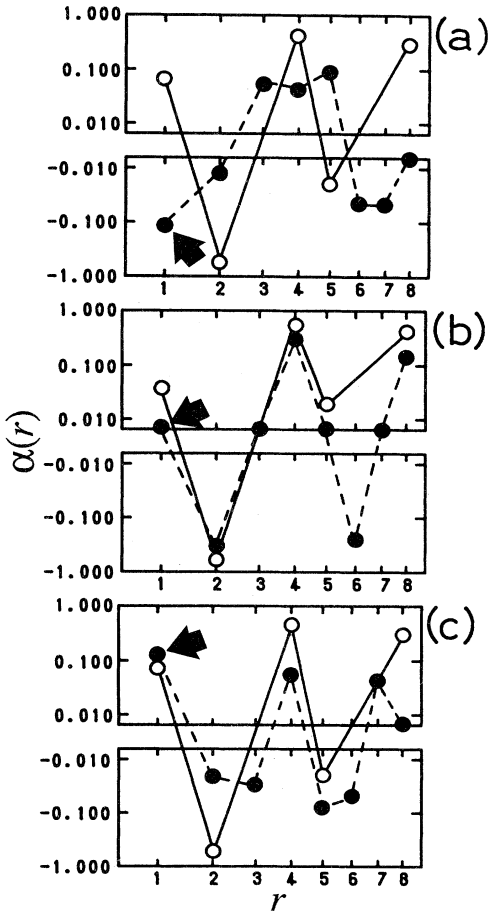

FIG. 3. Warren-Cowley parameters of the atomic arrangements corresponding to the spectra of Fig. 2. Open and closed circles indicate the degree of order for the (001) intraplanes and interplanes, respectively. Note that the value of $\alpha(1)$, which is the pair correlation of the 1NN atoms in the (001) interplane (indicated with an arrow), shows a systematic change with V_{1v}; (a) negative, (b) almost zero, and (c) positive.

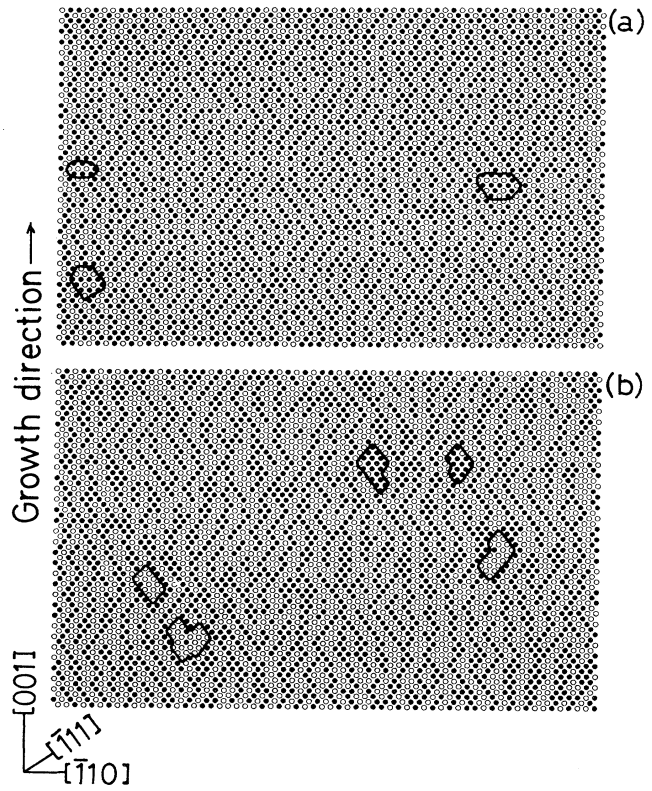

FIG. 4. (110) cross-sectional views of the configuration of A (○) and B (●) atoms in the epilayer corresponding to 1(a) and 1(c). In both, the CuPt-type-ordered structure shows a double periodicity along the $[1\bar{1}1]$ or $[\bar{1}11]$ direction. In addition, small regions with CuAu-I-type structures and like-atom clusters disperse in (a) $V_{1v}<0$ and (b) $V_{1v}>0$, respectively. (Some of these are enclosed.)

$\Delta\tau$ corresponds to an increase in the frequency of diffusing paths of atoms on the surface. Therefore, the long $\Delta\tau$ indicates high growth temperature or low deposition rate. There exist wavy diffuse streaks passing through the $\frac{\bar{1}}{2}\frac{1}{2}\frac{1}{2}$ and the $-(\frac{1}{2}-\delta),\frac{1}{2}-\delta,0$ ($\delta>0$) positions along the growth direction. Their shape and intensity maximum position change with the increase of $\Delta\tau$. The degree of curvature for the streak can be measured by δ, and the values of δ are (a) 0.08, (b) 0.07, and (c) 0.05. As compared with (a), the curvature of the streak in (c) is small. In other words, the wavy streaks appear in the early stage of ordering and the straight ones in the late stage. Such straight streaks are actually observed together with strong superlattice spots,[15–17] indicating the formation of well-developed ordered domains. In (a), the streaks have their intensity maximum position at $-(\frac{1}{2}-\delta),\frac{1}{2}-\delta,0$ ($\delta=0.08$). This result suggests the presence of periodicity with $2.4d_{1\bar{1}0}$ [$d_{1\bar{1}0}$: spacing of $(1\bar{1}0)$ lattice planes] along the $[1\bar{1}0]$ direction. The intensity maximum, on the other hand, shifts to the $\frac{\bar{1}}{2}\frac{1}{2}\frac{1}{2}$ positions characteristic of the CuPt-type order. These changes of streak due to the evolution of CuPt-type order are in good agreement with those obtained experimentally,[15,16] though we consider only the pairwise atomic interactions between the first and second neighboring atoms in the Ising model. Thus, our crystal-growth model includes an essential point for the ordering during the epitaxial growth.

We calculate the pair correlation of atoms in order to investigate the degree of order for an epilayer. Figure 6 shows Warren-Cowley parameters of the atomic arrangements corresponding to the spectra of Fig. 5. The pair correlation between the even neighboring atoms is gradually strong with increase in $\Delta\tau$, indicating the development of CuPt ordering in the epilayer. The absolute values of the Warren-Cowley parameter within the (001)

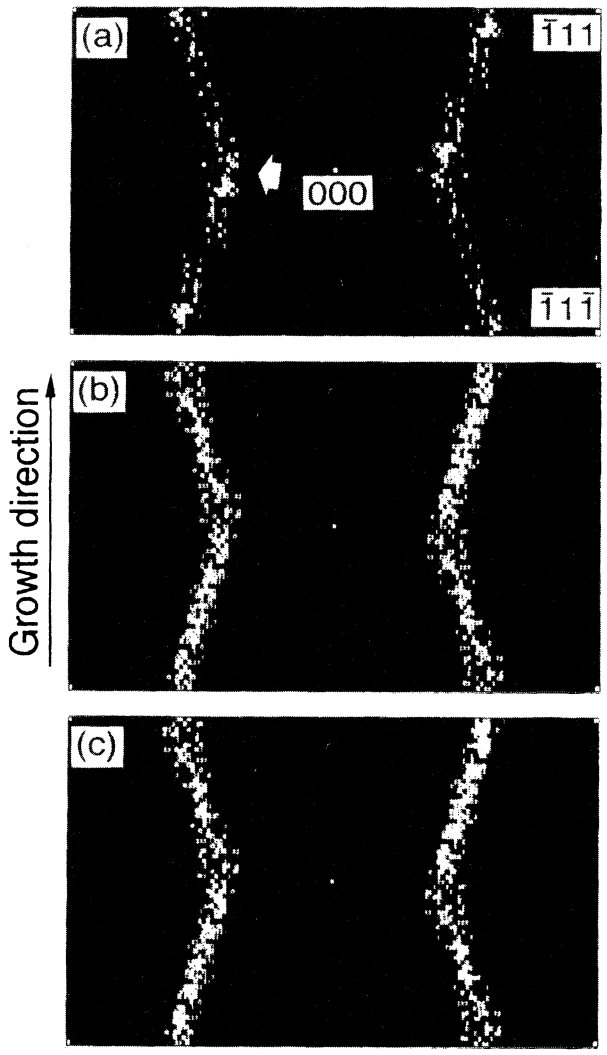

FIG. 5. (110) Fourier transforms of the atomic arrangements in epilayers as a function of stacking time interval $\Delta\tau$. (a) 20, (b) 100, and (c) 1000 MCS. The energy parameters except V_{2v} ($=-0.2|V_{1h}|$) are set to be the same as the ones used in the previous calculation shown in Fig. 2(c). Long $\Delta\tau$ corresponds to high growth temperature or low deposition rate. With the increase of $\Delta\tau$, the curvature of streaks becomes small and their intensity maximum position shifts from the vicinity of the fundamental lattice spot to the $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ position, as indicated by white arrows.

planes are larger than those of the (001) interplanes. That is, the ordering within the (001) planes is faster than that along the [001] direction, and this result suggests the appearance of platelike-ordered phases perpendicular to the growth direction. This phenomenon can be explained in terms of the pairwise atomic interaction, as follows. In the case of the CuPt-type ordering, the effective interaction which contributes the ordering of the (001) interplanes is V_{2v} only. The absolute value of V_{2v} set in the present simulation is much smaller compared with the growth temperature. Therefore, thermal fluctuation may easily disturb the ordering along [001]. On the contrary, the interactions of the (001) intraplanes are large enough to develop the ordered structure.

The values for the 1NN pairs of (001) interplanes in Fig. 6 are (a) 0.141, (b) 0.123, and (c) 0.066, being close to zero with the progress of ordering. This behavior suggests that the number and the size of like-atom clusters become small. As mentioned in Sec. III A, the slanting of the diffuse scatterings in (110) electron diffraction pattern is due to the existence of clusters of like-atoms among the CuPt-ordered domains. From the behavior of $\alpha(1)$ in Fig. 6, it was confirmed that there is a strong correlation between the curvature of streak and value of $\alpha(1)$. Note that the Warren-Cowley parameter for the 2NN interplane correlation, $\alpha(2)$, which is indicated by the arrow, takes a positive value in Fig. 6(a), and gradually changes into a negative value with an increase in $\Delta\tau$, as shown in (b) and (c). It seems that the behavior of $\alpha(2)$ relates to the change of the intensity maximum positions in the streak.

Figures 7(a) and 7(b) demonstrate (110) cross-sectional views of the atomic arrangements in the early and late stages of ordering, respectively. It is seen that numerous like-atom clusters appear in (a). When $\Delta\tau$ is short, the ordering on the surface proceeds incompletely, and the positive interaction V_{1v} allows the formation of small like-atom clusters. The epilayer thus obtained includes like-atom clusters which elongate along the [001] direction; accordingly the value of $\alpha(2)$ becomes positive. The spatial distribution of the clusters have a periodicity of $2.5d_{1\bar{1}0}$ along the $[1\bar{1}0]$ direction, and this result is in agreement with that of Fig. 5(a). The epilayer of Fig. 7(b) contains few like-atom clusters, and well-developed-

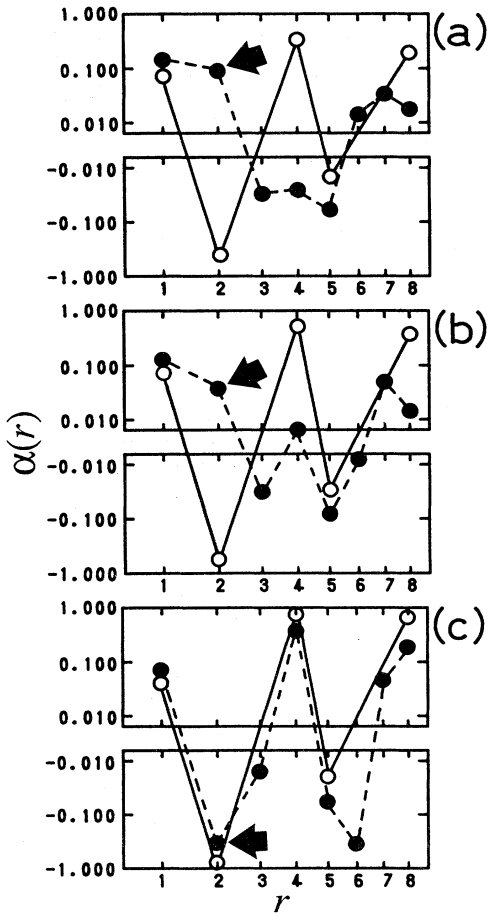

FIG. 6. Warren-Cowley parameters of the atomic arrangements corresponding to the spectra of Fig. 5. Open circles are of the pair correlation of atoms within the (001) planes, and closed ones are of the interplane correlation. The value of $\alpha(2)$, which is the pair correlation of the 2NN atoms in the (001) interplane, changes from a positive value to a negative value with the progress of ordering.

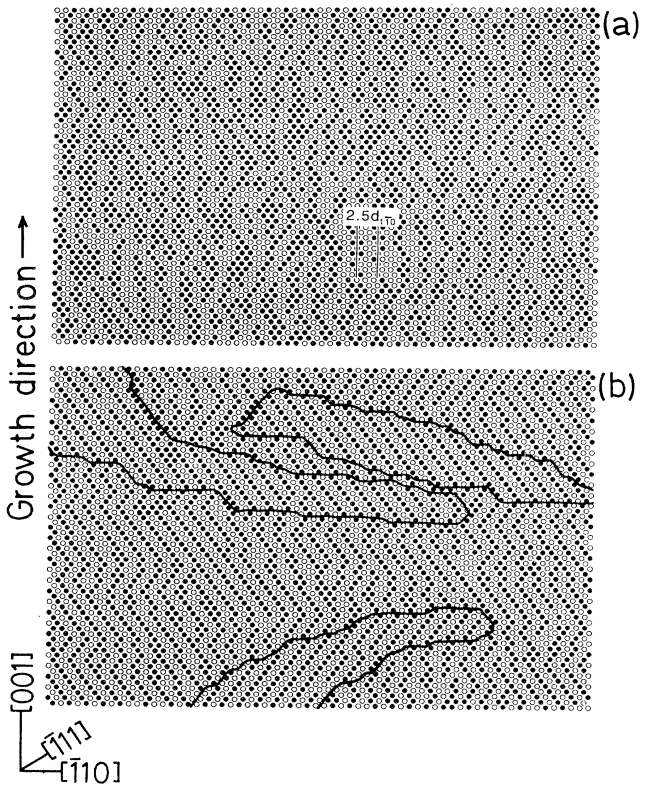

FIG. 7. (110) cross sections of the atomic arrangements corresponding to the spectra of 5(a) and 5(c). Stacking time interval $\Delta\tau$ for (a) and (b) is 20 and 1000 MCS, respectively. In (a), the epilayer contains many like-atom clusters that elongate along the growth direction. On the other hand, the CuPt-type-ordered domains perpendicular to the [001] direction appear in (b). Note that the $(\bar{1}11)$ and $(1\bar{1}1)$ domains incline toward the $[\bar{1}1\bar{1}]$ and $[\bar{1}11]$ directions from $[\bar{1}10]$, respectively.

ordered phases extend perpendicular to the growth direction. Therefore, $\alpha(2)$ takes a negative value with a large value for $\Delta\tau$ and the intensity maximum position in the diffuse streaks moves to the $\frac{\bar{1}}{2}\frac{1}{2}\frac{1}{2}$. It should be noted that the $(\bar{1}11)$ and $(1\bar{1}1)$ domains slightly tilt toward the $[\bar{1}1\bar{1}]$ and $[\bar{1}11]$ directions from $[\bar{1}10]$, respectively, and this result is in agreement with an experimental one.[19,31] The formation mechanism of the inclined domain has been already reported in our previous paper.[27(b)]

IV. CONCLUSION

Monte Carlo simulation based on an Ising-type model for the layer-by-layer epitaxial growth including surface migration of atoms has been carried out to explain features of diffuse scatterings and microstructures in partially ordered III-V semiconductor alloys. The findings of this investigation are as follows.

(1) An epitaxial layer obtained by the layer-by-layer stacking includes platelike CuPt-type-ordered domains with many (001) plane faults. These cause the diffuse scatterings running along the growth direction through peaks at the $\frac{\bar{1}}{2}\frac{1}{2}\frac{1}{2}$ positions in a (110) diffraction pattern.

(2) The shape of the diffuse streaks depends sensitively on the value of V_{1v}, which is for the interactions with 1NN atoms on the underlying plane. That is, the streaks are drawn toward the fundamental lattice spots for the case of positive V_{1v}, while they move away from the fundamental points for negative V_{1v}. The former shape is observed in the actual diffraction pattern, indicating that the value of V_{1v} should be positive in the III-V semiconductor alloys.

(3) The positive V_{1v} interactions form the dispersed small like-atom clusters among the CuPt-ordered domains. Our simulation demonstrates that the existence of them causes the wavy displacement of the streaks toward the fundamental reciprocal-lattice points.

(4) The shape of diffuse streaks and their intensity maximum positions depend upon the growth temperatures or deposition rates. An epilayer obtained by the low temperature or the high-growth rate contains numerous like-atom clusters elongating the [001] direction and wavy diffuse streaks have intensity maximum position around the fundamental lattice spots, $-(\frac{1}{2}-\delta),\frac{1}{2}-\delta,0$ $(\delta>0)$. With the development of ordering, well-developed ordered domains are formed and the position shifts toward the $\frac{\bar{1}}{2}\frac{1}{2}\frac{1}{2}$ and straight-shaped streaks appear.

ACKNOWLEDGMENTS

This study was supported by Grants-in-Aid for Scientific Research on Priority Areas "Crystal Growth Mechanism in Atomic Scale" (No. 03243107 and 04227107). One of us (S.M.) acknowledges the financial support of Nissan Science Foundation.

[1]P. Henoc, A. Izrael, M. Quillec, and H. Launois, Appl. Phys. Lett. **40**, 963 (1982).
[2]T. L. McDevitt, S. Mahajan, D. E. Laughlin, W. A. Bonner, and V. G. Keramidas, Phys. Rev. B **45**, 6614 (1992).
[3]A. G. Norman and G. R. Booker, J. Appl. Phys. **57**, 4715 (1985).
[4]O. Ueda, S. Isozumi, and S. Komiya, Jpn. J. Appl. Phys. **23**, L241 (1984).
[5]N. Kuwano, K. Fukuda, K. Oki, S. Tanaka, K. Hiramatsu, and I. Akasaki, J. Cryst. Growth **98**, 82 (1989).
[6]B. de Cremoux, P. Hirtz, and J. Ricciardi, in *Proceedings of the 8th International Symposium on GaAs and Related Compounds,* edited by H. W. Thim, IOP Conf. Proc. No. 56 (Institute of Physics and Physical Society, London, 1981), p. 115.
[7]G. B. Stringfellow, J. Cryst. Growth **58**, 194 (1982).
[8]K. Onabe, Jpn. J. Appl. Phys. **21**, 323 (1982).
[9]For a review, see G. B. Stringfellow, J. Cryst. Growth **98**, 108 (1989).
[10]A. Gomyo, T. Suzuki, K. Kobayashi, S. Kawata, and I. Hino, Appl. Phys. Lett. **50**, 673 (1987).
[11]T. Nishino, J. Cryst. Growth **98**, 44 (1989).
[12]S. R. Kurtz, L. R. Dawson, R. M. Beifeld, D. M. Follstaedt, and B. L. Doyle, Phys. Rev. B **46**, 1909 (1992).
[13]T. Kanata, M. Nishimoto, H. Nakayama, and T. Nishino, Phys. Rev. B **45**, 6637 (1992).
[14]T. S. Kuan, T. F. Kuech, W. I. Wang, and E. L. Wilkie, Phys. Rev. Lett. **54**, 201 (1985).
[15]A. Gomyo, T. Suzuki, and S. Iijima, Phys. Rev. Lett. **60**, 2645 (1988).
[16]D. S. Cao, E. H. Reihlen, G. S. Chen, A. W. Kimball, and G. B. Stringfellow, J. Cryst. Growth **109**, 279 (1991).
[17]P. Bellon, J. P. Chevalier, E. Augarde, J. P. Andre, and G. P. Martin, J. Appl. Phys. **66**, 2388 (1989).
[18]I. J. Murgatroyd, A. G. Norman, and G. R. Booker, J. Appl. Phys. **67**, 2310 (1990).
[19]C. S. Baxter, W. M. Stobbs, and J. H. Wilkie, J. Cryst. Growth **112**, 373 (1991).
[20]G. P. Srivastava, J. L. Martins, and A. Zunger, Phys. Rev. B **31**, 2561 (1985); **38**, 12 694(E) (1988); D. M. Wood and A. Zunger, *ibid.* **40**, 4062 (1989); R. Osorio, J. E. Bernard, S. Froyen, and A. Zunger, *ibid.* **45**, 11 173 (1992).
[21]P. Boguslawski, Phys. Rev. B **42**, 3737 (1990).
[22]C. H. Park and K. J. Chang, Phys. Rev. B **45**, 11 775 (1992).
[23]S. B. Ogale and A. Madhukar, Appl. Phys. Lett. **59**, 1356 (1991); **60**, 2095 (1992).
[24]N. Otsuka, Y.-E. Ihm, Y. Hirotsu, J. Klem, and H. Morkoc, J. Cryst. Growth **95**, 43 (1989).
[25]S. Matsumura, N. Kuwano, and K. Oki, Jpn. J. Appl. Phys. **29**, 688 (1990).
[26]S. Matsumura, K. Takano, N. Kuwano, and K. Oki, J. Cryst. Growth **115**, 194 (1991).
[27](a) M. Ishimaru, S. Matsumura, N. Kuwano, and K. Oki, J. Cryst. Growth **128**, 499 (1993); (b) Phys. Rev. B **51**, 9707 (1995).
[28]M. Ishimaru, S. Matsumura, N. Kuwano, and K. Oki, J. Appl. Phys. **77**, 2370 (1995).
[29]K. Kawasaki, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. G. Green (Academic, New York, 1972), Vol. 2.
[30]J. M. Cowley, J. Appl. Phys. **21**, 24 (1950).
[31]C. S. Baxter, R. F. Broom, and W. M. Stobbs, Surf. Sci. **228**, 102 (1990).

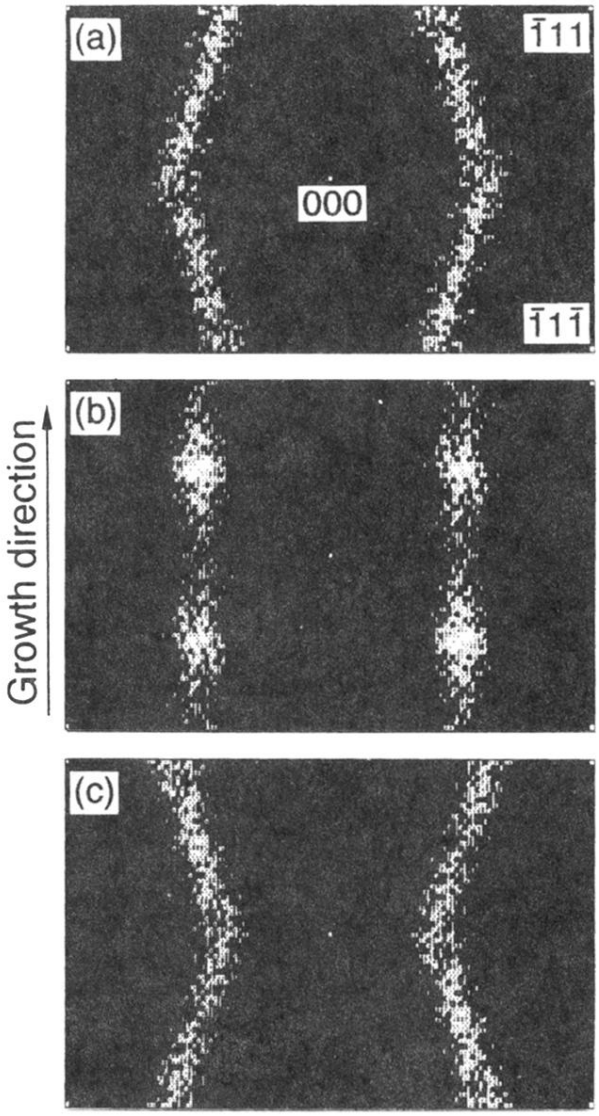

FIG. 2. (110) Fourier power spectra of the atom configurations in epilayers as a function of V_{1v}, which is for the interactions with 1NN atoms on the underlying plane. V_{1v} is equal to (a) $-|V_{1h}|(<0)$, (b) 0, and (c) $|V_{1h}|$ (>0), and the stacking time interval $\Delta\tau=20$ MCS. Diffuse streaks passing through the $\frac{\bar{1}}{2}\frac{1}{2}\frac{1}{2}$ and the equivalent positions appear along the growth direction, and their curvature depends on the sign of V_{1v}. The shape of streaks in (c) are in good agreement with that in the actual diffraction patterns reported previously.

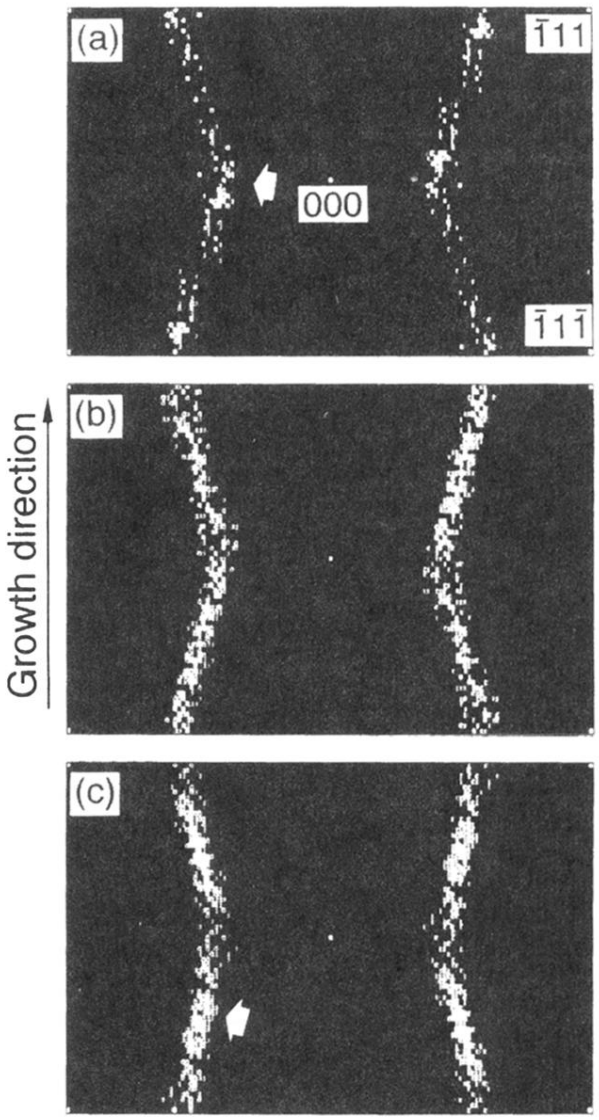

FIG. 5. (110) Fourier transforms of the atomic arrangements in epilayers as a function of stacking time interval $\Delta\tau$. (a) 20, (b) 100, and (c) 1000 MCS. The energy parameters except V_{2v} ($=-0.2|V_{1h}|$) are set to be the same as the ones used in the previous calculation shown in Fig. 2(c). Long $\Delta\tau$ corresponds to high growth temperature or low deposition rate. With the increase of $\Delta\tau$, the curvature of streaks becomes small and their intensity maximum position shifts from the vicinity of the fundamental lattice spot to the $\bar{\frac{1}{2}}\frac{1}{2}\frac{1}{2}$ position, as indicated by white arrows.