Atomic arrangements of a CuAu-I type ordered structure in strained $In_xGa_{1-x}As/In_yAl_{1-y}As$ multiple quantum wells

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Many investigations on ordered phases in various III–V ternary compound semiconductor epilayers have been performed during past many years [1–10]. Among the various kinds of the ordering structures, a CuPt-type superstructure has been the most extensively studied structures in III–V ternary semiconductors [1–10]. However, relatively little work has been done on the CuAu-I type ordering in comparison with a CuPt-type ordering [11]. An existence of the CuAu-I type ordering in the lattice-mismatched quantum wells provides an important physical information in achieving high efficiencies for optoelectronic devices. Even though some works concerning existence of a CuAu-I-type ordered structure in lattice-mismatched $In_xGa_{1-x}As/In_yAl_{1-y}As$ multiple quantum wells have been performed [11], studies concerning the atomic arrangements of a CuAu-I type ordered structure in lattice-mismatched $In_xGa_{1-x}As/In_yAl_{1-y}As$ multiple quantum wells (MQWs) are still important for understanding their detailed microstructural properties. Furthermore, lattice matched and lattice-mismatched $In_xGa_{1-x}As/In_yAl_{1-y}As$ quantum structures have been particularly attractive because of the considerable interest in both investigations of fundamental physical properties and fabrications of optoelectronic devices operating in the long wavelength spectral region [12–16].

This paper reports atomic arrangements of a CuAu-I type ordered structure in lattice mismatched $In_xGa_{1-x}As/In_yAl_{1-y}As$ MQWs grown by molecular beam epitaxy (MBE). Selected area electron diffraction pattern (SADP) measurements were performed in order to investigate the atomic and the ordered structures of lattice matched and lattice mismatched $In_xGa_{1-x}As/In_yAl_{1-y}As$ MQWs. Atomic arrangements of a CuAu-I type ordered structure are described on the basis of the SADP results.

The two kinds of samples with MQW structures used in this work were grown on S-doped (100)-oriented InP substrates by using MBE and consisted of the following structures: a 0.15-μm Be-doped ($p = 2 \times 10^{19}$ cm^{-3}) $In_{0.53}Ga_{0.47}As$ capping layer for ohmic contacts, a 1-μm Be-doped $In_{0.52}Al_{0.48}As$ cladding layer ($p = 1 \times 10^{18}$ cm^{-3}), a 700−Å undoped $In_{0.52}Al_{0.48}As$, 11 periods of undoped $In_xGa_{1-x}As$ ($t = 95$ Å)/In_yAl_{1-y} As ($t = 55$ Å) MQWs, a 0.6-μm Si-doped $In_{0.52}Al_{0.48}As$ layer ($n = 2 \times 10^{18}$ cm^{-3}), and 1-μm Si-doped InP buffer layer ($n = 2 \times 10^{18}$ cm^{-3}). The lattice-mismatched $In_xGa_{1-x}As/In_yAl_{1-y}As$ MQWs is $In_{0.46}Ga_{0.54}As/In_{0.55}Al_{0.45}As$ structure whereas the lattice-matched MQWs is a $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ structure. Among the p-i-n modulator structures, $In_xGa_{1-x}As/In_yAl_{1-y}As$ MWQs regions are important for achieving high-performance devices since they are active layers in modulators. The growth temperatures of the $In_xGa_{1-x}As$ and the $In_yAl_{1-y}As$ layers are 410 °C and 440 °C, respectively. The composition and the thickness of each layer in the $In_xGa_{1-x}As/In_yAl_{1-y}As$ MQWs were determined by double-crystal X-ray diffraction, photoluminescence, and cross-sectional TEM measurements.

Cross-sectional TEM specimens were prepared by forming a sandwich with epoxy, followed by mechanical cutting and polishing with diamond paper to an approximately 30 μm thickness, and then argon-ion milling at liquid-nitrogen temperature to electron transparency. High-resolution micrographs were obtained using a JEOL JEM 2000EX transmission electron

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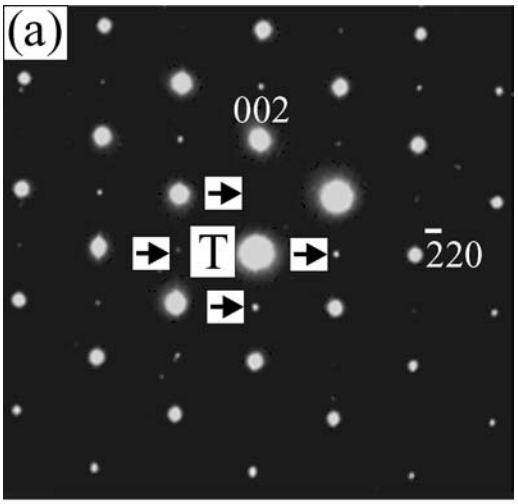

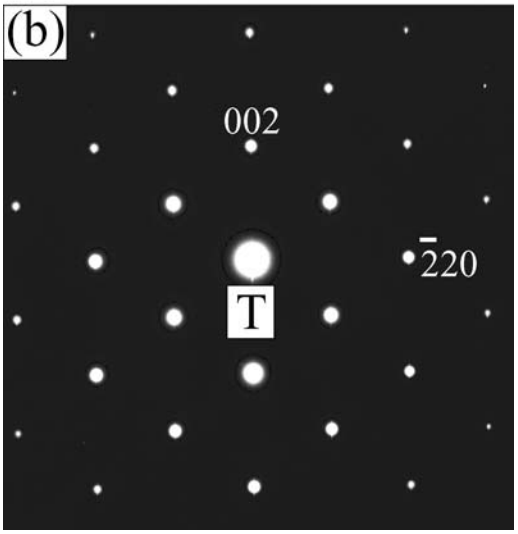

Figure 1 Selected area electron diffraction patterns of (a) the $In_{0.46}Ga_{0.54}As/In_{0.55}Al_{0.45}As$ multiple quantum wells, which shows {001} and {110} symmetry extra spots through the [110] projection, and (b) the $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ multiple quantum wells, which shows no extra spot.

microscope operating at 200 kV with a high-resolution pole piece.

Figs 1a and b show the SADPs from the $In_{0.46}Ga_{0.54}As/In_{0.55}Al_{0.45}As$ and the $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ superstructure regions through the [110] projection, respectively. Fig. 1b shows that the strong electron spots occur in a single pattern resulting from the lattice matching between the $In_{0.53}Ga_{0.47}As$ well and the $In_{0.52}Al_{0.47}As$ barrier. However, the SADP of the $In_{0.46}Ga_{0.54}As/In_{0.55}Al_{0.45}As$ superstructure region shows {001} and {110} asymmetry extra spots along the ⟨111⟩ direction together with the strong symmetric superstructure spots [11]. The superstructure spots are observed at the positions indexed by 001, $1\bar{1}0$, and $\bar{1}10$ in the $In_{0.46}Ga_{0.54}As/In_{0.55}Al_{0.45}As$ superstructure region, as shown in Fig. 1a. This particular set of the superstructure spots is attributed to the typical characteristics of the CuAu-I type ordered structure (1, 1, 0), which is generally reported in the III–V ternary systems [17–19]. Doublet periodicity exists in the CuAu-I type structure along the ⟨001⟩ and the ⟨110⟩ directions due to alternating cation and anion, {001}

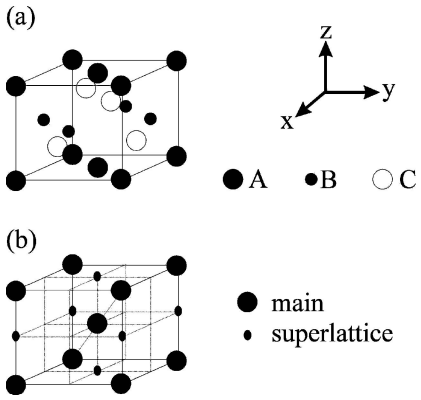

Figure 2 Schematic diagrams of (a) the real lattice and the reciprocal lattice of the CuAu-I type orderings.

and {110}, monolayers along the ⟨001⟩ and the ⟨110⟩ directions. The real lattice and the reciprocal lattice of the CuAu-I type ordering can be described in Fig. 2a and b, respectively. These ordered phases lead to a pattern of superstructure reflections with *hkl* indices, which are $h + k =$ even and $k + l =$ odd, as shown in Fig. 1a [18]. That is to say, the values of the *hkl* are (even, even, or odd) or (odd, odd, or even) in the [110] zone axis. The superstructure spots are nearly circular, which indicates that the ordering is almost periodic. Furthermore, the SADP taken from the lattice matched $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ superstructure corresponding to the region does not show extra spots related to the CuAu-I type ordering, as shown in the Fig. 1b.

Fig. 3 shows a schematic diagram of atomic arrangement of the CuAu-I type ordering at group III sublattice

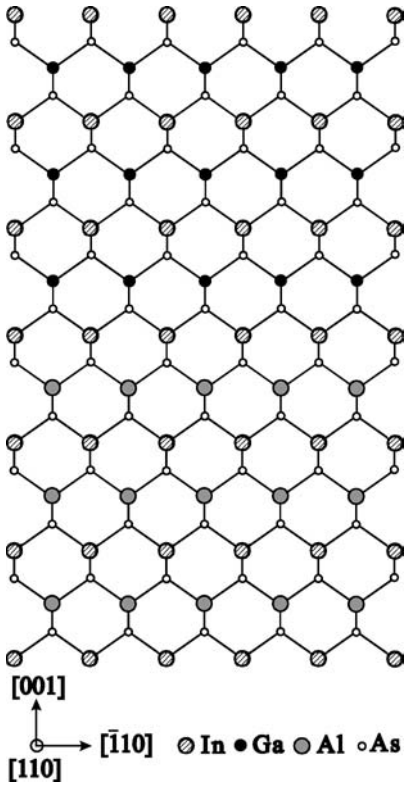

Figure 3 A schematic diagram of the atomic arrangement of the CuAu-I type structure in the $In_{0.46}Ga_{0.54}As/In_{0.55}Al_{0.45}As$ superstructure region.

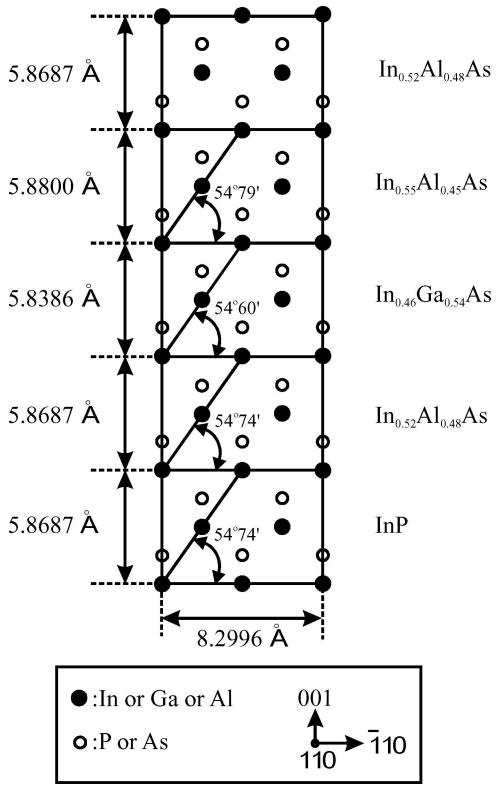

Figure 4 A schematic diagram of the (110) projection of the crystal structure for an $In_{0.46}Ga_{0.54}As/In_{0.55}Al_{0.45}As$ quantum well.

along the [110] projection. Even though In and Ga atoms or In and Al atoms in the typical disordered structure are randomly distributed at group III sublattices, and As for the group V sublattices, an atomic arrangement in the CuAu-I-type ordered structure forms a periodic arrangement of the {001} and the {110} layers, in the order of InAs/GaAs and InAs/AlAs sublattices along the [001] and the [110] layers, as shown in the Fig. 3. Thus, the composition of CuAu-I type ordered region is expected to be approximately $In_{0.5}Ga_{0.5}As$ or $In_{0.5}Al_{0.5}As$.

A possible schematic diagram of the (110) projection of the crystal structure for an $In_{0.46}Ga_{0.54}As/In_{0.55}Al_{0.45}As$ quantum well, taking into account strain effect, is shown in Fig. 4. The lattice constants described in Fig. 4 are derived from the bulk lattice constants assuming the elastic theory. The lattice constants of GaAs, InAs, AlAs, InP, $In_{0.57}Ga_{0.47}As$, and $In_{0.52}Al_{0.48}As$ are 5.6532, 6.0584, 5.6611, 5.8687, 5.8687, and 5.8687 Å, respectively, and those of the $In_xGa_{1-x}As$ active layers are determined by using the Vegard's law [23]. Fig. 4 shows the creation of an angle difference between the {111} planes due to pseudomorphic growth. The angles among the $In_{0.52}Al_{0.48}As$, $In_{0.46}Ga_{0.54}As$, and $In_{0.55}Al_{0.45}As$ planes originates from the difference in the perpendicular components of the lattice constants of the $In_{0.46}Ga_{0.54}As$ and $In_{0.55}Al_{0.45}As$ layers. The angles between the ⟨110⟩ and ⟨111⟩ directions for the $In_{0.52}Al_{0.48}As$, $In_{0.46}Ga_{0.54}As$, and $In_{0.55}Al_{0.45}As$ layers are 54.74 °C, 54.60 °C, and 54.79 °C, respectively. Thus, the $In_{0.46}Ga_{0.54}As$ and $In_{0.55}Al_{0.45}As$ layers have a pseudomorphic relationship with the $In_{0.52}Al_{0.48}As$ buffer layer. The values of the horizontal and vertical strains and the horizontal stress of the $In_{0.46}Ga_{0.54}As$ obtained from the relationship between the stress and strain components are 0.498×10^{-2}, -0.483×10^{-2}, and 5.16×10^{-2} dyne cm^{-2}, respectively, and the corresponding values for the $In_{0.55}Al_{0.45}As$ layer are -0.185×10^{-2}, 0.178×10^{-2}, and 0.178×10^{-2} dyne cm^{-2}, respectively. While the $In_{0.46}Ga_{0.54}As$ layers receive a tensile strain, the $In_{0.55}Al_{0.45}As$ layers receive a compress strain. Therefore, the existence of the CuAu-I type ordering in $In_{0.46}Ga_{0.54}As/In_{0.55}Al_{0.45}As$ superlattices originates from the strain compensation behavior between the $In_{0.46}Ga_{0.54}As$ and the $In_{0.55}Al_{0.48}As$ layers, which might be related to the localized ordering.

In summary, the results of the SADP measurements on the lattice mismatched $In_xGa_{1-x}As/In_yAl_{1-y}As$ superlattices showed the existence of a CuAu-I type ordered structure. The CuAu-I type ordered structure was observed in the periodically lattice-mismatched $In_{0.46}Ga_{0.54}As/In_{0.55}Al_{0.45}As$ heteroiterfaces. Possible atomic arrangements of the CuAu-I-type ordered structure in the lattice-mismatched $In_xGa_{1-x}As/In_yAl_{1-y}As$ MQWs were described on the basis of the SAPD results. These results can help improve understanding of the microstructural properties of the strained $In_xGa_{1-x}As/In_yAl_{1-y}As$ MQWs.

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