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Characterization of GaAs/AlAs Interface Structure by High Resolution Transmission Electron Microscopy

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By comparing Transmission Electron Microscopy (TEM) images and computersimulation images, we have shown that the brightness variation at the interface of a lattice image is a good indicator of the atomic configuration and atomic step structure at the GaAs/AlAs interface. On the basis of the obtained results, the growth temperature dependence of the interfacial configuration was studied. The height and density of the atomic step in a sample grown at 500°C are a monolayer (2.8 A) for each length longer than 100 A, while they are one or two monolayers (5.6 A) for each length less than 30 A for a sample grown at 700°C.

1. Introduction

With the aim of developing quantum effect such as resonant hot electron devices transistors (RHET)¹ and new materials including ordered alloys², much attension has paid to extremely thin been semiconductor/semiconductor (SC/SC)multilayers which contain many interfaces. The atomic resolution investigation of the interface configuration great is of importance, as the interface influences the optical and electronic properties of multilayer structures.

High-resolution transmission electron microscopy (HRTEM) is employed extensively in such investigations. Usually, the interface is studied by observing a cross section of the sample, with the electron beam parallel to the <110> direction. $^{3-7}$ The position of the interface on a micrograph is deduced from the difference in the background intensity of the lattice image. However, the background intensity is neither a reliable nor a sensitive indicator of the position of the SC/SC interface or its atomic configuration. $^{5-7}$ One way of studying the position of an interface is to use <100> direction lattice images. $^{5-7}$ However, <110> projection is preferable to <100> projection, because the widest lattice-spacing in the <100> direction, i.e. d_{200} =2.83A for GaAs, is shorter than that in the <110> direction, i.e. d_{111} =3.3A for GaAs. This makes the observation of the lattice-images in the <110> direction easier than that in the <100> direction.

Here. describe we one means of determining the atomic configuration at the GaAs/AlAs interface and its atomic step structure by using <110> direction TEM images. By comparing the TEM images and computersimulation images we can show that the brightness variation at the interface in the lattice image is a good indicator of the interface position .

2. Experiment

GaAs/AlAs SLs with 9-by-9 atomic layers were grown for 60 periods on (001)-oriented GaAs substrates by conventional molecular beam epitaxy (MBE) at substrate temperatures of 500°C (sample A) and 700°C (sample B). The preparation of the samples prior to TEM is essentially the same as that used by Lidbury et al.⁸ The TEM apparatus used is an Akashi EM-002B operating at 200 kV with a spherical aberration coefficient of 0.4 mm and a chromatic aberration coefficient of 0.8 mm. The Sherzer defocus⁹ is about -380 A and the point-to-point resolution power about 1.8 A.

3. Results and Discussion

3.1 Lattice images

Figure 1 shows a cross-section TEM lattice image of a GaAs/AlAs superlattice grown at 700°C. The growth direction is from bottom to top, as indicated in the figure. This image was taken at a defocus of about - 300 A under [110] axial illumination. The thickness of the TEM sample is less at the bottom than at the top.

In Figure 1 one white dot corresponds to one molecule of GaAs or AlAs due to a lack in the resolution (the projected distance between Ga and As, or Al and As is 1.4 A while the TEM resolution is 1.8 A).

We can use the background intensity to distinguish between the GaAs and AlAs layers -- black for GaAs and white for AlAs. 3-6 The difference in the background intensity in GaAs and AlAs closely depends on the sample Contrast is intensified at some thickness. appropriate thicknesses as is clearly shown in region B of Figure 1. However, it is difficult to accurately determine the interfacial atomic configuration from the background intensity. Therefore, we concentrated on the arrays formed at the interfaces by the brightest spots, indicated by the arrows in Figure 1.

The bright spots have the following features.

 They appear on one side only of the two AlAs/GaAs and GaAs/AlAs interfaces.

(2) The clarity of the spots depends on the thickness of the sample. They can be observed

clearly in regions A and C, but not in region B. (3) They form an array corresponding to one monolayer. Doubling of arrays is sometimes observed, together with a stepped interfacial configuration.

To clarify the origin of the brighter spots and determine the atomic configuration at the interface we had to use computer calculation.

3.2 Computer simulation images

We ran a computer simulation of the HRTEM lattice image using Cowley-Moodie multislice methods^{10, 11} with the parameters listed in Table 1, using FACOM VP-200 and VP-400 supercomputers. A superlattice is composed of an alternating stack of nine GaAs monolayers and nine AlAs monolayers with an atomic step structure on one side of the two interfaces. A large unit cell was constructed. It included 18 monolayers in the [001] direction (growth direction), 30 monolayers in the [110] direction, and two monolayers in the [110] direction (electron beam direction).

Figure 2 shows the through-focus images of the simulated lattice images of the 64 Athick GaAs/AlAs superlattices, together with the actual lattice arrangement. The defocuses are (a) -300 A, (b) -380 A, (c) -460 A, and (d) -540 A. A monolayer step is situated at the interface of the lower side of the AlAs layers (lower interface).

Figure 3 shows the thickness dependence of the simulated lattice images for a defocus of -460 A. The thicknesses are (a) 40 A, (b) 80 A, (c) 120 A, (d) 160 A, and (e) 200 A. A monolayer step is at the interface of top side in AlAs layers (top interface).

The dependence of the background intensity on the sample thickness is clearly shown in Figure 3. This dependence corresponds to the changes of the (0 J/18 0) $J=\pm1$, ±3 , ±5 , ..., satellite-reflection intensity.³, 12 From this result, we estimate the thickness of the TEM sample to be about 100 to 150A at region B of Figure 1.

For the arrays of bright spots at the interfaces, our computer simulation revealed: (1) They belong to the AlAs layer rather than the GaAs layer. The asymmetric appearance on one side of two interfaces is caused by the asymmetric alignment of the Al and Ga atoms at the two interfaces. 5

(2) They are particulary marked when the sample thickness is between 60 and 80 A at the Sherzer focus.

(3) They are intensified by under-focusing about 100 A from the Sherzer focus.

(4) We can read the atomic step structure on the upper interface more easily than that on the lower interface because the bright spot arrays are a good indicator of the step structure.

In consequence, it can be said that an arrays of bright spots in the lattice image is a good means of accurately obtaining the position of the interface and the atomic configuration.

4. Growth temperature dependence of the interfacial configuration in SLs

MO studied the difference in the interfacial configuration between sample A (grown at 500°C) and B (grown at 700°C), using TEM as shown in Figures 4(a) and (b), respectively. The thickness of these samples is about 60 to 100 A, as estimated from the background intensity of the GaAs and AlAs layers and from the appearance of the bright spots.

For the SL grown at 500° C, the arrays of bright spots corresponding to one monolayer is observed over a range wider than 100 A along the interface, as shown in Figure 4(a). From this, we can estimate that the height and density of the atomic steps are one monolayer (2.8 A) for each length longer than 100 A.

On the other hand, the height and density

Table 1. Values of parameters used in the computer simulations.

Accelerating voltages	E=200 kV	
Lattice parameter	a=5.66 A	
Slice thickness	z=√2 a	
Numbers of beams	72581	
Divergence angle	$\alpha = 6 \times 10^{-4}$	rad
Spherical aberration coefficient	Cs=0.4 mm	
Chromatic aberration constant	∆=41.6 A	



Fig. 1. A cross-sectional TEM lattice image of the GaAs/AlAs superlattice grown at 700°C.

(a) -300 A (b) -380 A (c) -460 A (d) -540 A	(e) model
Fig. 2. Through-focus images of lattice images of the 64 A-thick superlattices, and the actual arrangement.	simulated GaAs/AlAs lattice



Fig. 3. Thickness dependence of the simulated lattice images for a defocus of -460 A.

are one or two monolayers (5.6 A) for each length less than 30 A for the SL grown at 700°C, because the single array of bright spots extends for only 30 A and many doubling arrays are observed. A possible reason for the doubling of arrays is that some arrays at different positions on the interface overlap when observed along the $[1\overline{10}]$ direction. This is caused by the dominant step distance being shorter than the sample thickness, which allows overlapping to occur.

We can, therefore, find out directly that the sample grown at 500°C has an interface with fewer steps than that grown at 700°C.

5. Conclusion

We have studied a means of determining the atomic configuration at the GaAs/AlAs interface and its atomic step structure by using <110> direction TEM images. An arrays of the bright spots in the TEM lattice image is used as an indicator of the interfacial configuration. We can estimate the height and density of the atomic steps to be one monolayer (2.8 A) for each length longer than 100 A for a superlattice grown at 500°C, one or two monolayers (5.6 A) for each length less than 30 A for one grown at 700°C.

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Fig. 4. Growth temperature dependence of the interfacial configuration in GaAs/AlAs superlattices. (a) 500°C, (b) 700°C.

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