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Compositional grading in GaAsSb grown on GaAs substrates

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ABSTRACT

The composition profile and lattice strain of GaAsSb grown on GaAs substrates by molecular beam epitaxy have been investigated using the Rutherford backscattering spectrometry (RBS) and X-ray reciprocal space mapping. Through RBS, we found that the Sb content in the layer increases from the interface to the top surface. The X-ray reciprocal space mapping shows that the GaAsSb lattice also gradually relaxes as the layer becomes thicker. The behavior of composition grading and gradual lattice relaxation is quite different from those of III–V ternary compounds with two group III atoms.

1. Introduction

Semiconductor heterostructures based on GaAsSb/GaAs material system [1,2] have attracted much attention in recent years due to the potential applications in electronic and optoelectronic devices such as heterojunction bipolar transistors (HBTs) [3–5] and laser diodes [6–8]. Adding Sb in the base of a typical InGaP/GaAs HBT or an AlGaAs/GaAs HBT can effectively reduce the turn-on voltage and the power dissipation of the transistor. The use of GaAsSb/GaAs heterostructure can also make 1.3 μm emission possible for laser diodes made on GaAs substrates. But because GaAsSb, which has a larger lattice constant than GaAs, contains two different group V atoms, controlling the composition of the layer with uniform distribution is not easy. For layers grown by molecular beam epitaxy (MBE), the relative amount of As and Sb in the film does not necessarily depend on the flux ratio of the two elements because the sticking coefficients of these two group V elements are less than one. When the grown film is under strain, as in the case of GaAsSb/GaAs heterostructures, the incorporation of As and Sb can depend on the amount of strain in the film.

In this work, the GaAsSb layer grown on GaAs was studied using the Rutherford backscattering spectrometry (RBS) and X-ray reciprocal space mapping (RSM). These two techniques allowed us to determine the strain and composition profiles of the GaAsSb layer. We found that there is a naturally formed Sb gradient in the layer to accommodate the strain caused by the lattice difference between GaAs and GaAsSb.

2. Experiment

The samples were grown on (001) n-type GaAs substrates by a Veeco GEN II solid-source MBE system. The group V species of As_2 and Sb_2 were controlled by cracker cells with needle valves. The growth temperature was monitored by an infrared pyrometer. A GaAs buffer layer of 200 nm was first grown at 580 °C to smooth out the surface before the growth of the GaAsSb layer. Six samples with different GaAsSb thicknesses (10, 30, 40, 60, 90, and 200 nm) were prepared. They were all grown at the same condition, i.e., the same growth temperature (500 °C) and other fabrication process. The As_2 and Sb_2 sources were used with the same beam equivalent pressure (beam flux) for the constituent elements. The growth rate was 0.65 ML/s for all samples. The samples were then characterized by X-ray measurements and RBS. The X-ray diffraction and RSM measurements were conducted using Cu-Kα radiation in a Bede D1 system; the RBS was performed using 4 MeV C^{2+} or 2 MeV He^{+} ions. Backscattered particles were detected at an angle of 160° with respect to the incident beam.

3. Results and discussion

X-ray RSM around the asymmetrical GaAs (224) diffraction spot was performed to estimate the degree of lattice relaxation and Sb

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composition of the GaAsSb layers. Fig. 1 shows the RSM results for these samples with the GaAsSb layer of (a) 10 nm, (b) 30 nm, (c) 90 nm, (d) 200 nm. The main diffraction spots, which correspond to GaAs (224) and GaAsSb (224), were marked in the figures. The vertical axis (z axis) represents the direction normal to the sample surface and the horizontal axis (x axis) is in the [110] direction. So the horizontal location of a diffraction spot tells us the lateral lattice spacing, while the vertical location tells us the lattice spacing along the layer growth direction. For a cubic lattice without any strain, the (224) diffraction spot in the reciprocal space should have a q_z/q_x ratio of $\sqrt{2}$ [9]. We can see from these figures that the spot location of the GaAs substrate remains the same and follows this rule, but the location of the GaAsSb spot deviates from this unstrained (total relaxed) condition and changes as the layer thickness is changed.

When GaAsSb is 10 nm thick, we can see from Fig. 1(a) that the two diffraction spots have the same lateral position but very different vertical positions. This indicates that the in-plane lattice constant of the GaAsSb layer is the same as that of the GaAs substrate. In other words the GaAsSb layer is fully strained. When the GaAsSb layer becomes thicker, the diffraction spot of GaAsSb moves away from the fully strained position and to a smaller q_x value and a larger q_z value, and at the same time the spot becomes fuzzier and more widely spread. So the strain in the GaAsSb layer is gradually relaxed as the grown layer becomes thicker. But the relaxed lattice of GaAsSb has a wide spread of lattice spacing, indicating the residual strain is not uniform. Based on the location of the diffraction spot of GaAsSb on RSM, we can find the relationship between its Poisson ratio and the (relaxed) lattice constant. Then from Vegard's law, we can calculate the Sb composition and the amount of lattice relaxation in the GaAsSb layer. Fig. 2 shows the degree of lattice relaxation and the Sb content as functions of the GaAsSb thickness. We need to mention that the data points shown in the figure were calculated from the brightest spots in the diffraction patterns. So they represent the average values of the layers. From the intensity contour of the pattern, we can see that the brightest spots are close to where the highest Sb content is. As will be pointed out next, they are close to the surface of the layer.

To study the depth profile of Sb composition in the GaAsSb layer, we used RBS with 4 MeV C^{2+} or 2 MeV He^{+} ions [10,11]. Based on the Rutherford differential scattering cross section, the backscattering yield obtained from a given target atom increases

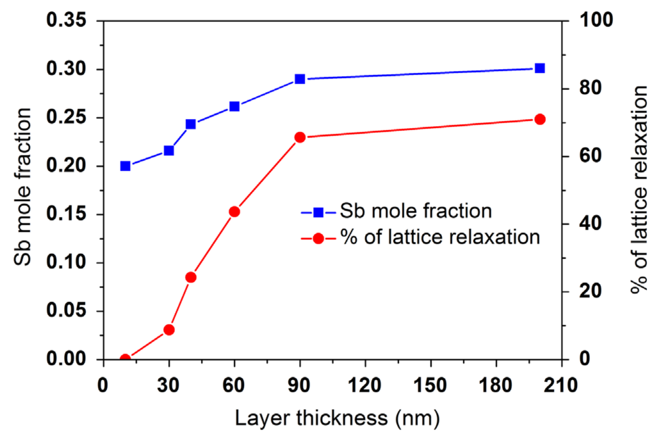

Fig. 2. The Sb composition and amount of relaxation of the GaAsSb layer in the samples with various GaAsSb thicknesses.

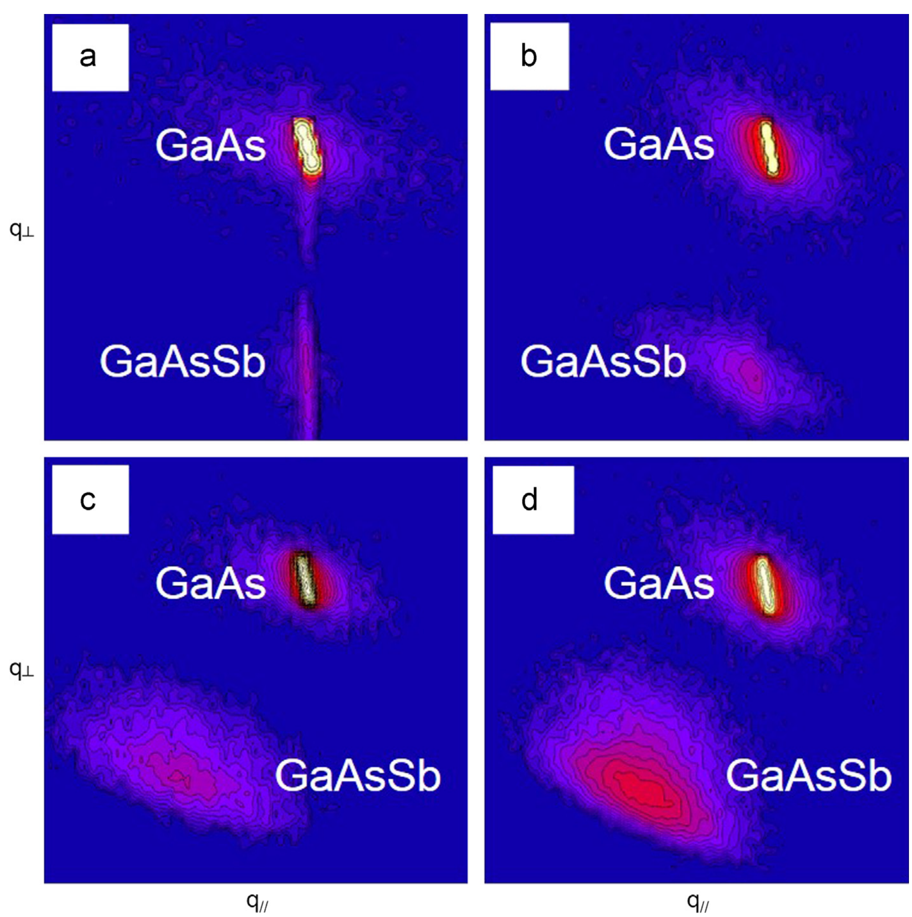

Fig. 1. RSM measurements taken at the GaAs (224) reflection for the samples with the GaAsSb buffer layer of (a) 10 nm, (b) 30 nm, (c) 90 nm, (d) 200 nm.

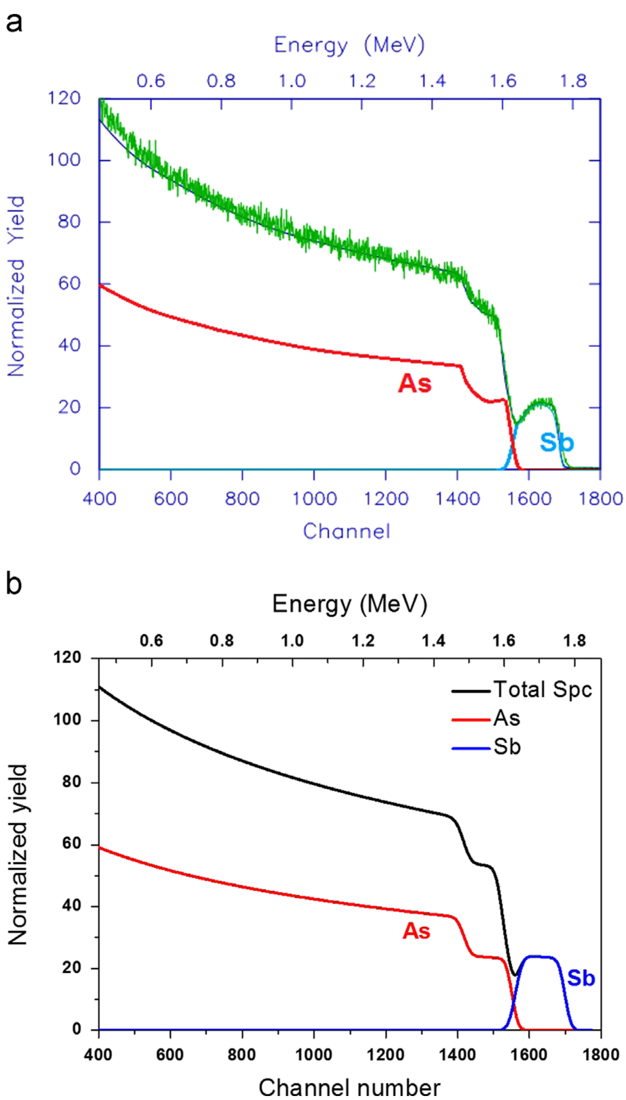

Fig. 3. (a). The experimental RBS spectrum of the sample with the GaAsSb layer of 200 nm. Using computer simulation, we were able to decompose the spectrum into those of the constituent elements, As and Sb, as also shown in this figure and Fig. 3(b). The random RBS spectra from simulation for the sample with the same GaAsSb thickness. The Sb composition keeps constant throughout the GaAsSb epitaxial layer.

with the atomic number (ion mass) of the incoming beam. So heavy ions such as C provide much better resolution than normally used light ions such as protons and alpha particles [12]. All samples were characterized by RBS with the use of heavy ions except one with the GaAsSb layer of 200 nm, which was measured using RBS with the light ions. Fig. 3(a) shows the RBS spectrum of the sample with a 200 nm GaAsSb layer. Using computer simulation, we were able to decompose the spectrum into those of the constituent elements as also shown in Fig. 3(a). We found from simulation that the Sb composition gradually increase toward the surface. This can also be seem from the As distribution near the surface. The As signal tapers down from the GaAs/GaAsSb interface to the surface, indicating the gradual increase of the Sb content in the layer. For comparison, we did a simulation for a hypothetical GaAsSb layer on GaAs with uniform Sb distribution. The Sb content was assumed to be 30% and the thickness was 200 nm, which is the same as that of the sample used in Fig. 3(a). The calculated RBS spectrum along with the As and Sb signals for this ideal sample are shown in Fig. 3(b). Clearly, the RBS yields from the As and Sb atoms in the GaAsSb layer show plateau regions in the spectrum.

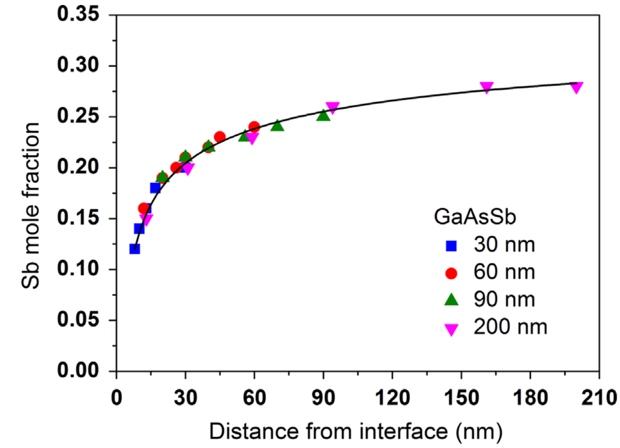

Fig. 4. The grading profile of the Sb content in the GaAsSb layer with various thicknesses.

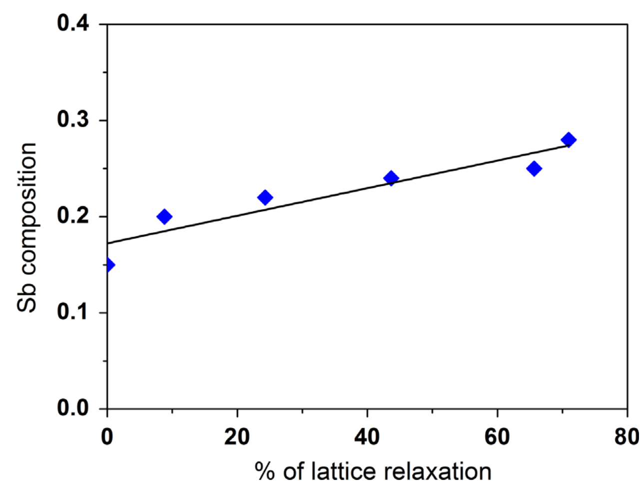

Fig. 5. The Sb content as a function of the percentage of lattice relaxation in the GaAsSb layer.

This is the result of the uniform composition distribution in the layer. In contrast, the real sample had a gradual change in the composition.

Fig. 4 shows the calculated Sb distribution for samples with different GaAsSb thicknesses. The distribution of Sb in the layer increases as we move away from the substrate/epilayer interface and all data points from different samples fall on the same curve. Different from the growth of strained ternary compounds with two group III elements, where the distributions of the group III elements are uniform, the incorporation of the group V elements depends on the thickness of the layer and how far it is from the interface. From the Sb distribution shown in Fig. 4 and the strain in the layer, we can plot the Sb content as a function of the percentage of lattice relaxation in the layer. The result is shown in Fig. 5. Approximately a straight line relationship was obtained. The vertical interception indicates that ~17% of Sb can be incorporated in the layer without causing lattice relaxation. Above that (thicker layer), both the Sb mole fraction and the degree of lattice relaxation increase at the same time.

There are several factors that can influence the incorporation of Sb in the layer grown on a substrate that has different lattice constant. The Sb flux determines the amount of Sb when the layer is totally relaxed. In the initial stage of growth, the lattice has to align with that of the substrate. To reduce the strain energy, the actual amount of Sb that is incorporated in the layer is greatly reduced. As the growth continues, the increased strain elongates the lattice spacing in the vertical direction. The increased cell volume makes the incorporation of Sb easier, so more Sb is found in the layer. When the strain reaches a critical value, the lattice relaxes and the cell volume continues to increase as the lateral lattice spacing becomes wider. So the Sb incorporation continues to rise. Eventually the amount of Sb in the layer has to reach a steady state value determined by the beam flux as the layer is totally relaxed.

4. Conclusion

RBS using MeV C^{2+} or He^{+} ions and X-ray RSM measurements were used to study the chemical concentration and the lattice strain of GaAsSb grown on GaAs substrates. Whether we used the heavy or light ions, we were able to clearly observe the difference in the Sb composition inside the GaAsSb layer through the RBS spectra. It is found that the Sb composition fraction grades increasingly instead of keeping constant throughout the GaAsSb epitaxial layer. This is quite different from the growth of ternary compounds with two group III elements, which are generally uniform in the layer. The results from the X-ray RSM measurement also confirmed the results from the RBS experiment.

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