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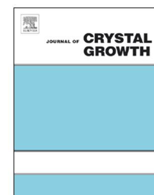

Molecular beam epitaxy of ErGaAs alloys on GaAs (0 0 1) substrates

Ri Guo Jin [a], Shuhei Yagi [a], Yasuto Hijikata [a], Shigeyuki Kuboya [b], Kentaro Onabe [b], Ryuji Katayama [c], Hiroyuki Yaguchi [a,*]

[a] Graduate School of Science and Engineering, 255 Shimo-Okubo, Sakura-ku, Saitama University, Saitama 338-8570, Japan
[b] Department of Advanced Materials Science, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan
[c] Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan

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A B S T R A C T

We have successfully grown high crystalline quality ErGaAs alloy layers by solid-source molecular beam epitaxy. The X-ray diffraction (XRD) peak of ErGaAs alloys was found to shift systematically from the GaAs peak with increasing Er concentration up to 3.7%. XRD (1 1 5) reciprocal space map measurements revealed that the ErGaAs epitaxial layer is coherently grown on GaAs. We found from XRD results that ErGaAs alloys with low Er concentrations tend to crystallize in the zincblende structure.

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1. Introduction

Erbium doped semiconductors have been attracting much attention because of their emission wavelength around 1.5 μm corresponding to the optical communication wavelength range [1,2]. Since the magnetic moment of rare-earth elements plays acts as the microscopic magnet, the magnetic properties of Er doped semiconductors have been also investigated [3,4]. Tanaka and Mishima [3] found from the magneto-optical spectra that there is little hybridization of *4f* and *sp* orbitals in (Ga, Er)As in contrast with the strong *sp*–*d* hybridization in (Ga, Mn)As. They also reported that no visible systematic shift from the peak due to GaAs was observed for the X-ray diffraction (XRD) profiles of (Ga, Er) As films with an Er concentration of 7.7×10^{20} cm^{-3}. Morinaga et al. [4] reported that Er^{3+} ions in GaAs provide little effect on the magnetic and magneto-transport properties even when the Er concentration is 2×10^{19} cm^{-3}. In the present study, we have successfully grown high crystalline quality ErGaAs alloy epitaxial layers by molecular beam epitaxy (MBE), and found that the XRD peak of ErGaAs layer shifts systematically from the GaAs peak with increasing Er concentration up to 8.1×10^{20} cm^{-3}.

2. Experimental procedure

The samples investigated were grown on undoped GaAs (0 0 1) substrates by solid-source MBE. After the surface oxide was removed at 590 °C, a 200-nm-thick GaAs buffer layer was grown at 570 °C. Next, a 460-nm-thick ErGaAs epitaxial layer was grown at the same temperature, and then capped by a 15-nm-thick GaAs layer. The Er cell temperature was changed between 1040 °C and1200 °C in order to obtain various Er fluxes. The structural properties of grown ErGaAs layers were investigated by high-resolution XRD. Secondary ion mass spectrometry (SIMS) was used to evaluate the Er concentration in ErGaAs layers. We also observed the surface morphology of the samples using an atomic force microscope.

3. Results and discussion

The surface morphology of the grown samples was observed by atomic force microscopy and the surface roughness was found to be approximately 2 nm. Fig. 1 shows the XRD 2θ–ω (0 0 4) scan profiles obtained from ErGaAs layers grown on GaAs (0 0 1) substrates with Er cell temperatures of 1040 °C, 1100 °C, 1150 °C and 1200 °C. The XRD peak of ErGaAs (0 0 4) is found to shift systematically from the GaAs (0 0 4) peak to lower angles with increasing Er cell temperature. This result contradicts with the previous report [3] although the reason is not clear. Concerning samples with a clear ErGaAs (0 0 4) peak, the full widths at half maximum of the peak were 60 and 150 arcsec for Er cell temperatures of 1150 and 1200 °C, respectively, indicating that the fluctuation in the lattice parameter becomes larger with increasing Er concentration. In order to obtain the experimental results presented below, we used mainly the ErGaAs grown with an Er cell temperature of 1150 °C because the XRD peak is the narrowest for this sample. The full width at half maximum of the XRD (0 0 4) rocking curve was 70 arcsec for the ErGaAs layer grown with an Er cell temperature of 1150 °C, which indicates that the crystalline quality of the ErGaAs layer grown in this study was considerably high.

Fig. 2 shows the SIMS profile of Er atoms in the sample grown with an Er cell temperature of 1150 °C. Secondary ion intensities for Ga and As are also shown in this figure. It is found from the depth profile that Er atoms were homogeneously distributed in

* Corresponding author Tel./fax: +81 48 858 3841.
E-mail address: yaguchi@opt.ees.saitama-u.ac.jp (H. Yaguchi).

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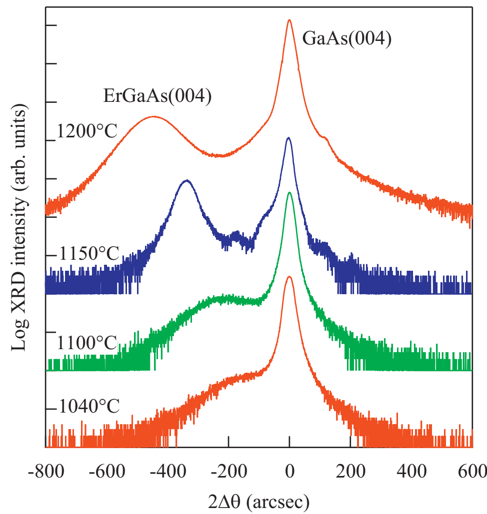

Fig. 1. XRD 2θ–ω (0 0 4) scan profiles obtained from ErGaAs layers grown on GaAs (0 0 1) substrates with Er cell temperatures of 1040 °C, 1100 °C, 1150 °C, and 1200 °C.

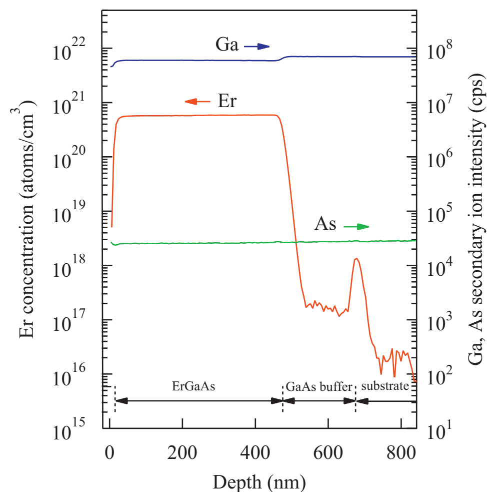

Fig. 2. SIMS profile of Er atoms in the sample grown with an Er cell temperature of 1150 °C. Secondary ion intensities for Ga and As atoms are also shown.

the ErGaAs epitaxial layer. The erbium concentration was found to be 5.8×10^{20} cm^{-3}, that is $x=2.7\%$. On the assumption that the lattice constant follows the Vegard's law, the Er concentration in the sample grown with an Er cell temperature of 1200 °C was estimated to be 8.1×10^{20} cm^{-3}, that is $x=3.7\%$. In addition, we found that the Er concentration is proportional to the flux ratio $f_{Er}/(f_{Er}+f_{Ga})$ at lower concentrations while a sublinear dependence on the flux ratio is shown at higher concentrations, where f_{Er} and f_{Ga} are Er and Ga fluxes, respectively. This indicates that the immiscibility becomes more pronounced between ErAs and GaAs because of the difference in the stable crystal structure with increasing Er concentration.

As can been seen from this figure, the Er concentration is found to decrease toward to the surface in the GaAs cap layer and no accumulation of Er is observed on the surface, indicating that the surface segregation of Er atoms is not so remarkable, although several papers [5,6] have suggested the importance of surface segregation when incorporating Er atoms into semiconductors. The secondary ion intensity of gallium in the ErGaAs layer was lower than that in the GaAs buffer layer and substrate, while the intensity for As was almost constant all over the sample. This shows that Er atoms are predominantly substituted for Ga atoms and thus incorporated in the epitaxial layer. Incidentally, there exists a spike of Er concentration at the interface between the GaAs buffer layer and substrate. This is attributed to the unintentional doping of Er because the cell temperature was elevated at 1150 °C during the oxide removal even though the shutter was closed.

Fig. 3 shows the XRD (1 1 5) reciprocal space map of the sample with an Er concentration of $x=2.7\%$. The solid curve in this figure indicates the coherent growth of epitaxial layers on GaAs. Since the peak of the ErGaAs (1 1 5) diffraction is on this line, the ErGaAs epitaxial layer obtained is coherently grown on GaAs. Assuming that the elastic constants of ErGaAs are the same as those of GaAs, we evaluated the relaxed lattice constant of ErGaAs at 0.5660 nm from the XRD results. In addition, the lattice constant of ErAs was estimated to be 0.5922 nm from the linear extrapolation based on the Vegard's law. This value is considerably larger than the lattice constant of ErAs with the rock salt structure (0.5743 nm). First-principles calculations predict that the lattice constant of ErAs with the zincblende structure is larger than that with the rock salt structure, although the details are not presented in this paper. These suggest that ErGaAs alloys with low Er concentrations tend to crystallize in the zincblende structure while ErAs crystallizes in the rock salt structure.

In order to further examine whether the crystal structure of ErGaAs alloys grown in this study is the zincblende structure or the rock salt structure, we measured the XRD intensity for (1 1 1) and (2 2 2) planes. Fig. 4 (a) and (b) show the XRD 2θ–ω (1 1 1) and (2 2 2) scan profiles of ErGaAs layers grown with an Er cell temperature of1150 °C, respectively. As can be seen from these figures, it is noticed the XRD intensity of ErGaAs (2 2 2) is particularly weak. In fact, the ratio of the integrated intensity is

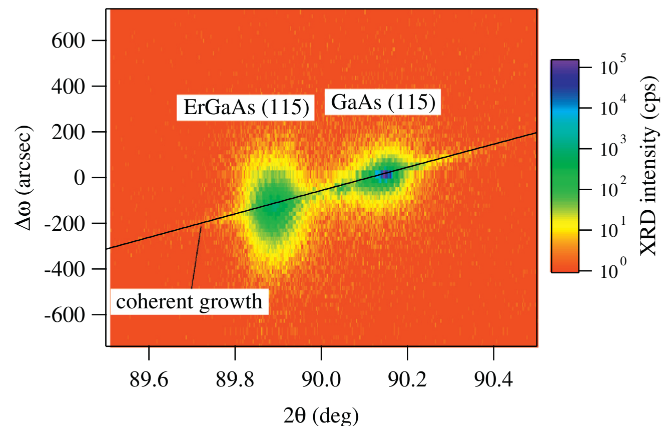

Fig. 3. XRD (1 1 5) reciprocal space map of the sample with an Er concentration of $x=2.7\%$.

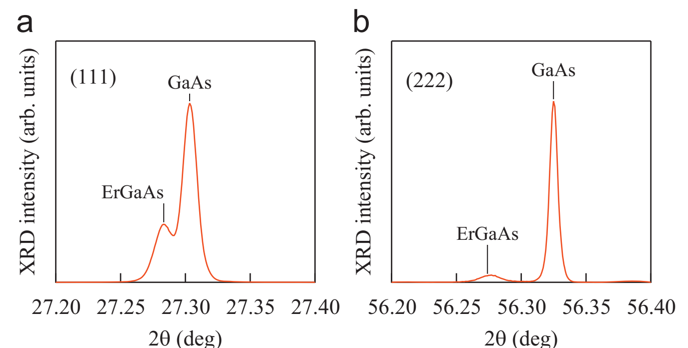

Fig. 4. XRD 2θ–ω (1 1 1) and (2 2 2) scan profiles of ErGaAs layers grown with an Er cell temperature of 1150 °C.

found to decrease from $I_{ErGaAs(1\ 1\ 1)}/I_{GaAs(1\ 1\ 1)}=0.42$ to $I_{ErGaAs(2\ 2\ 2)}/I_{GaAs(2\ 2\ 2)}=0.09$.

The crystal structure factor F_{AB} of the compound AB for the (2 2 2) diffraction plane is given by $4(f_A-f_B)$ if the crystal structure is the zincblende structure and by $4(f_A+f_B)$ for the rock salt structure, where f_A and f_B are atomic scattering factors for atoms A and B, respectively. This shows that the (2 2 2) XRD intensity for the zincblende structure is weaker than that for the rock salt structure because the XRD intensity is proportional to $|F_{AB}|^2$. Thus, the weak XRD intensity of ErGaAs for the (2 2 2) plane is attributed not to the rock salt structure but to the zincblende structure.

4. Conclusions

We have successfully grown ErGaAs alloy epitaxial layers on GaAs (0 0 1) substrates by solid-source MBE. The XRD 2θ–ω (0 0 4) peak due to ErGaAs alloy layers was found to shift systematically from the GaAs peak to lower angles with increasing Er concentration up to 3.7%. The XRD (1 1 5) reciprocal space map measurements revealed that the ErGaAs epitaxial layer is coherently grown on GaAs. It is found from the XRD results that ErGaAs alloys with low Er concentrations tend to crystallize in the zincblende structure.

Acknowledgements

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