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Lattice sites of diffused gold and platinum in epitaxial ZnSe layers

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Abstract

The lattice location of diffused gold and platinum in zinc selenide (ZnSe) epitaxial layers was studied using the Rutherford backscattering (RBS) channeling technique. Thin Au and Pt films were evaporated onto ZnSe samples. The Au/ZnSe samples were annealed at 525°C and the residual Au film was removed by etching. Channeling angular scan measurements showed that about 30% of Au atoms were close to substitutional site (displaced about 0.2 Å). In the case of the Pt/ZnSe samples the annealing temperatures ranged from 600°C to 800°C. The Pt minimum yields along ⟨1 0 0⟩ direction were close to the random value, varying from 80% to 90%. The measured Pt angular scans along ⟨1 0 0⟩ and ⟨1 1 0⟩ directions indicated a random location.

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1. Introduction

Initial efforts to develop short-wavelength diode lasers had focused on zinc selenide (ZnSe) which has a large band gap needed for blue or green lasing. Since then much research has been done to make a commercial blue green laser diode. One crucial task in this work is the preparation of ohmic contacts. Multilayer structures consisting of different metals, for example, Au, Pt, Te, Ti, Ni or Pd are used to obtain ohmic contacts with a small contact resistance [1,2].

The thermal stability of the contact structure is an important factor in designing the device structures and opitimization of their performance. The diffusion of contact metals, Au [3] and Pt [4], in ZnSe epitaxial layers on GaAs has been studied previously in our laboratory.

In this work we have studied the lattice location of diffused Au and Pt in ZnSe using the Rutherford backscattering (RBS) channeling technique. No studies concerning the lattice location of diffused metal atoms in ZnSe matrix have been published previously.

2. Experimental

2.1. Sample preparation

The studied samples were epitaxial ZnSe layers grown by molecular beam epitaxy on (1 0 0) GaAs

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substrate at Tampere University of Technology. Thin Au (100 nm) and Pt (10 nm) films were evaporated onto the samples.

The Au/ZnSe samples were annealed for 21 h in an argon atmosphere at 525°C. The residual Au film was removed by etching in a mixture of potassium iodide (KI) and iodine (I_2). After etching the sample was reannealed at 525°C for 5 h. The aim of this sample preparation procedure was to obtain a low concentration diffusion profile of Au near the ZnSe surface. The resulting Au concentration near the surface was 1–2 at.%. The Pt/ZnSe samples were annealed in an argon atmosphere at 600–800°C. The annealing times ranged from 40 min to 9 h. The Pt concentrations in the studied depth intervals near the surface region were 1–7 at.%. Etching of the Pt rich layer on the surface was not done because of the lack of a suitable etchant.

2.2. Channeling measurements

The RBS channeling measurements were carried out with a 2.5 MeV $^4He^+$ ion beam supplied by the 2.5 MV Van de Graaff accelerator at the University of Helsinki. The beam was collimated by slits and apertures resulting in a beam divergence of about 0.015°. Backscattered ions were detected in a solid state detector (acceptance angle about 11 msr) placed at an angle of 170° relative to the beam direction. A beam chopper system was used to measure the ion flux. The samples were placed in a 3-axis goniometer having an angular resolution of 0.05°. All measurements were performed in room temperature.

Channeling angular scans, i.e., the yield as a function of tilt angle along ⟨1 0 0⟩, ⟨1 1 0⟩ and ⟨1 1 1⟩ axial directions ere measured for the Au diffused ZnSe sample. The azimuthal angle between the scan plane and (1 1 0) plane was 22° in case of the ⟨1 0 0⟩ axial scan and 15° for the ⟨1 1 0⟩ and ⟨1 1 1⟩ scans. For the Pt diffused samples the minimum yields along ⟨1 0 0⟩ direction were measured for all the samples and angular scans along ⟨1 0 0⟩ and ⟨1 1 0⟩ axial directions were measured for the sample annealed at 800°C.

3. Data analysis and results

3.1. Au/ZnSe

In Fig. 1 the measured and simulated angular scans for diffused Au and ZnSe are presented. The simulations were performed using the Monte Carlo program Flux [5]. As can be noted the minimum yields in the measured ZnSe dips were higher than typical values in an undamaged lattice. Therefore, in the ZnSe simulation a 10% random

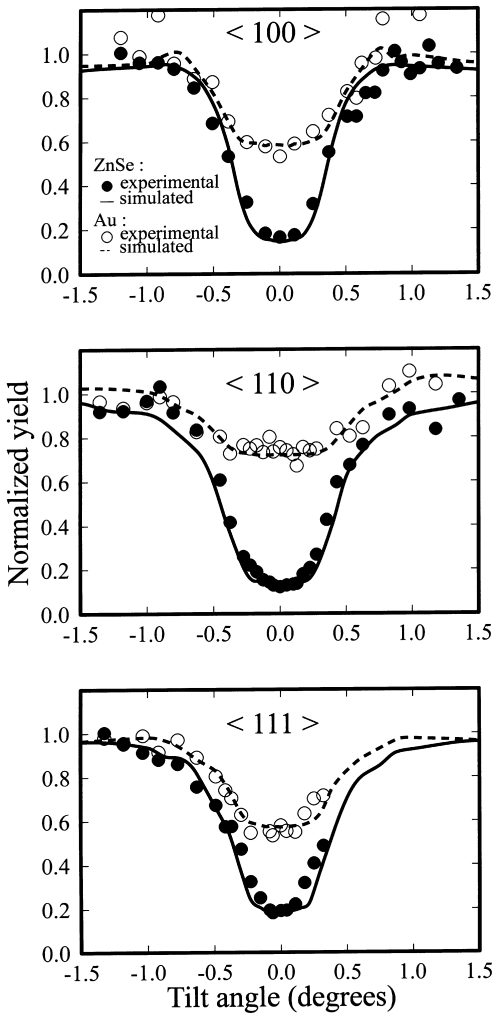

Fig. 1. Angular scans along ⟨1 0 0⟩, ⟨1 1 0⟩ and ⟨1 1 1⟩ directions in gold diffused ZnSe. A comparison between experimental and simulated results is shown.

fraction was added in all three scans. The Debye temperature of 200 K for the ZnSe lattice in the simulations was adopted.

The lattice site of Au atoms was determined by comparing the experimental angular scans with the simulated results corresponding to different Au atom sites. A large fraction of Au atoms was not on regular lattice site. Therefore, a constant background of 60% of the random value was added to the simulated results. The measured ⟨1 1 0⟩ and ⟨1 1 1⟩ dips for Au were narrower than the simulation for Au in substitutional sites indicating a small displacement. Therefore, it was most likely that the Au atoms were displaced along the ⟨1 0 0⟩ direction. The best correspondence with the measured results was obtained by taking 30% of Au atoms displaced 0.2 Å along the ⟨1 0 0⟩ direction.

The correspondence between experimental and simulated results (Fig. 1) was fairly good. In the experimental data the shape of the shoulders in the angular scan differs from the simulated shape in some cases. It seems like the angular scans were measured slightly off-axis.

The errors in the experimental results were about 5% due to statistical errors, uncertainties in ion flux monitoring and random yield determination used in normalization of the measured yields. The random fraction in the ZnSe dips was not taken into account in the Au dip analysis, i.e., Au dips were simulated as if the lattice was undamaged. Therefore, the total uncertainty in the fraction of displaced atoms and in the length of the displacement was about 20%. In the analysis it was assumed that Au atoms occupy only one regular lattice site. It was not possible to detect a possible small interstitial fraction (<5%) because of its small effect on the shape of the channeling angular scan and statistical error in the experimental data.

3.2. Pt/ZnSe

Fig. 2 shows the comparison of channeled and random spectra measured in Pt diffused samples annealed at temperatures 700°C and 800°C. The spectra were normalized to a common ion flux. Only a small difference between the Pt profiles can be noted. In the spectra for sample annealed at

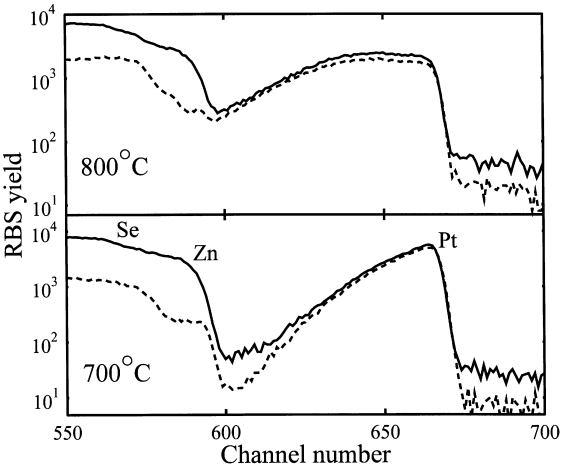

Fig. 2. RBS spectra obtained in random and along ⟨1 0 0⟩ direction with two Pt diffused ZnSe samples with annealed at temperatures of 700°C and 800°C.

700°C the larger difference in the Pt profile tail is due to a higher background level in the spectrum measured in random direction. The Pt minimum yields as high as 80–90% were observed along the ⟨1 0 0⟩ direction. The relatively high ZnSe minimum yield (about 30% in ⟨1 0 0⟩ direction) indicated a poor crystal quality. In the sample annealed at 800°C, the Pt minimum yield determined at high Pt concentration region near the surface was found to be lower than that of the low Pt concentration region deeper in the lattice. This was due to dechanneling in the damaged layer. The

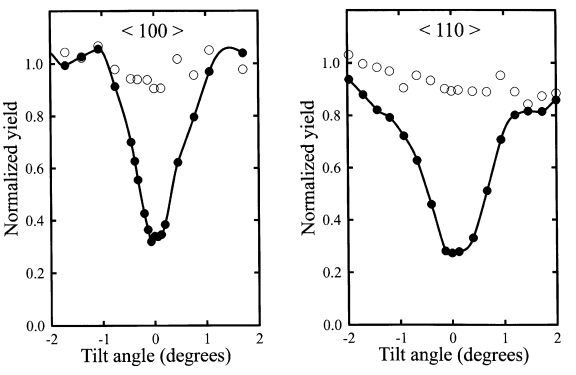

Fig. 3. Experimental angular scans along ⟨1 0 0⟩ and ⟨1 1 0⟩ directions for a platinum diffused ZnSe sample (annealing temperature 800°C). The solid lines are drawn to guide the eye.

minimum yield for the sample annealed at 700°C did not vary significantly in the studied depth interval.

The angular scans along the ⟨1 0 0⟩ and ⟨1 1 0⟩ directions were measured for the sample annealed at 800°C. For this sample the Pt minimum yield was found to be the lowest. As can be noted from the Fig. 3, these angular scans indicated that Pt atoms did not occupy any particular sites.

4. Discussion

Lattice location of Au has been determined in other semiconductor materials, for instance, in CdTe [6] and in silicon [7]. In both cases a fraction of Au atoms was found to be near the substitutional lattice site. Au is likely to be a substitutional impurity in the ZnSe lattice because Au is a monovalent atom and can act as an acceptor in ZnSe while substituting Zn in the lattice [8]. The results obtained in this study comply with this known behaviour. The Au atoms near the substitutional site were found to be slightly displaced. This could be due to formation of small clusters or pair formation of vacancy and Au atom [9].

In the Pt diffused samples the Pt concentration near the surface was too high for lattice location determination. One possible solution to this problem would be removing of the surface layer for instance by sputtering.

Because of the high Pt concentrations it was not possible to compare the Pt lattice site results with the Au case. Theoretically, a larger difference in electronegativities exist between Pt and Zn and Se than between Au and the host atoms. Therefore, Pt atoms should not as likely occupy substitutional sites as Au atoms in ZnSe.

To conclude, about 30% of Au atoms occupied substitutional sites. The substitutional Au atoms in ZnSe were found to be slightly displaced along ⟨1 0 0⟩ direction. The rest of the Au atoms were distributed randomly. In the case of Pt atoms in ZnSe no specific lattice site was observed.

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