

STRUCTURAL PROPERTIES OF INTERFACES IN AlInAs/GaAs SUPERLATTICES

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The structural investigation of AlInAs/GaAs superlattices has been performed using high resolution X-ray diffraction and X-ray reflectivity. The samples differing each other in the In content and in the number of bilayers were grown by MOCVD on GaAs (001) substrates with a miscut in the range from 0° to 3°. The combination of the above mentioned X-ray techniques allows to characterise the morphology of interfaces. The system chosen provides us effects strong enough in both diffraction and reflection modes. The reciprocal space maps were obtained in both modes, in the diffraction one In reflections 004 and 002, always in various azimuths.

The investigation revealed well-defined lateral periodicity of the interfaces. We suppose the interfaces are constituted from step-like objects, formed during growth through bunching of the miscut-induced monolayer steps on the substrate surface. The elementary cell of this twodimensional structure is a parallelogram. We compared the experimental results with theoretical calculations performed on the simple basis of coherent scattering by point centres lying at the interface. It follows from the results, that the shape of bunch steps depends strongly on the In concentration. This is in agreement with our experimental findings. For higher In concentration the misfit dislocations occur and relaxation takes place. The maxima of the resonance diffuse scattering appear in the reflection experiments and due to relaxation they are not observed in the diffraction mode.

Keywords: X-RAY DIFFRACTION X-RAY REFLECTIVITY SUPERLATTICE**STUDY OF Si_{1-x}Ge_x/ Si-MBE GROWTH PROCESS BY USING AN *IN-SITU* ELLIPSOMETRIC MEASUREMENT**

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Much attention has been paid to SiGe layers on Si substrates for electronic device applications recently. The growth mechanism of the layer is very complicated because of the existence of the strain due to the lattice mismatch of about 4.2% between Si and Ge. This strain makes a strong influence on the growth mode, such as the Stranski-Krastanov growth, in which the layer-by-layer growth changes to the island growth to release the strain energy above the critical thickness of the layer. In this study we investigated the growth process of the SiGe layers using an ellipsometry and a Reflection High Energy Electron Diffraction (RHEED) *in-situ*. The ellipsometry gives us the informations not only about the growth surface, but also from the whole part of the growth layer. The Si_{1-x}Ge_x (x = 0.15, 0.30, 0.50) layers were grown on Si(111) substrates with 7x7 surface structure by a solid-source Molecular Beam Epitaxy (MBE) method at the substrate temperature of 520°C for 30,000 seconds. The ζ - δ curves obtained during the MBE growth varied significantly, representing the inhomogeneity of the growth layers. The detailed analyses of the ζ - δ diagram by the 3-points analysis method [1] showed that the refractive index of the growth layer increased in the initial stage of the growth and became almost constant when the thickness increased. The RHEED pattern exhibited streak patterns during the growth, showing that a smooth surface was always kept. This result indicates that the lattice strain is gradually relaxed during the growth.

References

[1] Yoshioka et al., Jpn.J.Appl.Phys. 40(2001)371-375.

Keywords: SIGE MBE ELLIPSOMETRY**APPLICATION OF POWDER DIFFRACTION METHODS TO THE ANALYSIS OF THE ATOMIC STRUCTURE OF NANOCRYSTALS: THE CONCEPT OF THE APPARENT LATTICE PARAMETER (alp)**S. Stelmakh¹ B. Palosz¹ S. Gierlotka¹ R. Pielaszek¹ E. Grzanka^{1,2} U. Bismayer³ H.-P. Weber⁴ W. Palosz⁵

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Application of conventional tools for elaboration of diffraction data of nanocrystals may lead to erroneous conclusion. An alternative approach, based on the so-called 'apparent lattice parameter' (alp) is introduced. We assume a model of nanocrystal having a grain core with well-defined crystal structure, surrounded by a surface shell with the atomic structure similar to that of the core but being under strain. The two components, the core and the shell, form a composite crystal with interfering, inseparable diffraction properties. Consequently, a set of lattice parameters used for characterization of simple crystal phases is insufficient for a proper description of the complex structure of nanocrystals.

We developed a method of evaluation of diffraction data of nanocrystals, which refers to a core-shell model and is based on the 'apparent lattice parameter' methodology. The models are defined by the lattice parameter of the core, thickness of the shell, and the magnitude and distribution of the strain field in the shell, Fig.1. for a given diffraction pattern, the alp values are calculated for every individual Bragg reflection. By modeling atomic structures of nanocrystals and calculating diffraction patterns we showed, that alp-Q plots show characteristic shapes which can be used for evaluation of the atomic structure of the core-shell system. We show, that using a model of nanocrystal with spherical shape and centro-symmetric strain at the surface shell we obtain theoretical alp-Q values, which match the plots determined experimentally for SiC, GaN, and diamond nanopowders.

Keywords: NANOCRYSTALS, SURFACE STRUCTURE, DIFFRACTION**STRUCTURE AND THERMAL STABILITY OF ULTRA-THIN DIFFUSION BARRIERS FOR COPPER METALLIZATION**

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Due to its higher electromigration resistance and lower electrical resistivity, copper has replaced aluminum as metallization material for integrated circuits. As copper is very mobile in metals and semiconductors, effective barriers to prevent the copper diffusion are needed. Tantalum can be used for this purpose. At elevated temperatures, however, the grain boundaries of this polycrystalline material are paths for fast copper diffusion. One possibility to improve the barrier stability is the application of amorphous films. In this work, the microstructure and thermal stability of 10 nm Ta-Si-N films capped with 50 nm copper layers were investigated. For different nitrogen flows, the barrier layers were reactively sputtered from a Ta₅Si₃ target onto thermally oxidized silicon. Using X-ray diffraction (XRD), X-ray reflectometry (XRR), glow discharge optical emission spectroscopy (GDOES), and transmission electron microscopy (TEM), we investigated the samples after different thermal treatments. In the as-deposited states, the structure of the Ta-Si-N films is an amorphous one, which is indicated by the appearance of diffuse maxima in the diffraction diagrams. The Bragg reflections of the polycrystalline copper show a predominating <111> fibre texture. With increasing nitrogen content, structural changes of the Ta-Si-N layers occur. To investigate the thermal stability of the samples, heat treatments were carried out at 873 K for different annealing times. The observed structural changes were found to depend sensitively on both the copper and the barrier layer. In the case of the Ta-Si film, tantalum diffusion to the sample surface already starts during the 1 h anneal, and first signs of barrier crystallization into Ta₅Si₃ are visible after thermal treatment for 4 h. With rising nitrogen content, the barrier stability increases. Even after annealing for 100 h, the Ta-Si-N layer with about 50 % nitrogen does not show any signs of crystallization.

Keywords: THIN FILMS, DIFFUSION BARRIERS, X-RAY DIFFRACTION