Strain relaxation mechanisms in hexagonal and cubic nitride heterostructures grown by plasma-assisted molecular beam epitaxy

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Due to the relatively large mismatch between GaN and AlN (about 2.7%), the issue of strain relaxation is of particular importance in the case of (Al,Ga,N) heterostructures in the hexagonal and cubic phase.

In the specific case of plasma-assisted molecular beam epitaxy, it will be shown that the strain relaxation occurs either plastically or elastically depending on various parameters such as growth temperature and metal/N ratio.

As a matter of fact, the problem of plastic relaxation is rather poorly investigated in the literature for nitrides. As a first step to adress the case of the hexagonal phase, X-ray reciprocal maps were used to determine the strain state of AlN layers grown on GaN templates. Correlatively, the AlN in-plane lattice parameter, as measured by RHEED, was followed during growth. The good agreement between the in-situ and ex-situ experiments led us to devise a model for the kinetics of strain relaxation whereby dislocations are not mobile. Indeed, for hexagonal nitrides grown along the c axis, the slip planes are such that it is unlikely for dislocations to move down to the interface plane under the action of the misfit bi-axial strain. Secondly, the precise determination of the strain state of the AlGaN epilayers in the whole composition range allowed us to draw — in a graph of thickness vs. composition — a border line between strained and (partly) relaxed conditions. This yields an experimental determination of the critical thickness for plastic relaxation which we have compared to those deduced from the existing models.

These studies were applied to the case of GaN/GaAlN and AlN/AlGaN superlattices in the hexagonal phase, which are used as Bragg mirrors. X-ray reciprocal maps and $\theta - 2\theta$ recordings were used to determine the strain state of the superlattice and the thickness of the individual layers. Correlatively, their strain state was calculated by applying, for each of the individual layers of the superlattice, our model for strain relaxation with a critical thickness deduced from our experimental curve. A good fit was obtained, allowing to precisely monitor and optimise the properties of these Bragg mirrors that are to be used in VCSEL structures.

The elastic strain relaxation mode is found to occur at high temperature. To illustrate this relaxation mode, the case of GaN/AlN heterostructures in both hexagonal and cubic phase has been investigated. In both cases, it is shown that the growth of GaN on AlN occurs according to a Stranski-Krastanow growth mode, i.e. that 3D islanding is observed after deposition of a bidimensional wetting layer [1]. The nucleation mechanism of the islands, their size and shape have been studied by AFM and TEM.

The optical properties of the islands were studied by cathodo- and photoluminescence. As concerns the dots in the hexagonal phase, the presence of a huge internal field of several MV/cm results in a very strong red shift of the photoluminescence

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energy. Then, for dots higher than 3 nm, the photoluminescence was observed below the energy gap of hexagonal GaN [2]. As a result of the 0 D character of the islands, the photoluminescence intensity was found to be practically independent of the temperature.

In the case of GaN dots with cubic structure, in which no internal field is present, the photoluminescence was always observed above the energy of the gap. It was found to depend on the total amount of GaN deposited, which is related to the size of the dots. Similar to the case of the hexagonal phase, the photoluminescence intensity was practically independent on the temperature, as a clear signature of the 0 D character of the islands.

We conclude that the strain relaxation of the nitrides is rather complex, varying from plastic to elastic as a function of the lattice mismatch and of the growth conditions. The control of the elastic strain relaxation mode (i.e. the Stranski-Krastanow growth mode) leads to the formation of quantum dots exhibiting a very strong and temperature independent photoluminescence in wavelengths ranging from UV to visible, depending on the size of the dots and on their cristallographic phase, i.e. hexagonal or cubic.

The controlled growth of such quantum dots opens the way to the realization of quantum dots-based lasers with low threshold current.

[1] B. Daudin, F. Widmann, G. Feuillet, Y. Samson, M. Arlery, J. L. Rouvière, Phys. Rev B **56**, R7069 (1997)

[2] F. Widmann, J. Simon, B. Daudin, G. Feuillet, J. L. Rouvière, N. T. Pelekanos, G. Fishman, Phys. Rev B **58**, R15989 (1998)