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Report:

GaN and related III-N compound semiconductors possess unique material properties which make them extremely attractive for optoelectronic and high temperature, high power microelectronic applications; they are the subject of great current interest, for example for the realization of blue-violet diode lasers. All the devices which have been fabricated up to now are based on heterostructures, whose fundamental parameters are the band discontinuities at the heterojunctions. In the present experiment we have studied the local structure at one such heterostructure, i.e. GaN on AlN(0001), with the aim of obtaining information on intermixing and strain of the epilayer. These experiments are part of an ongoing research program; we have previously studied GaN/SiC epilayers [1].

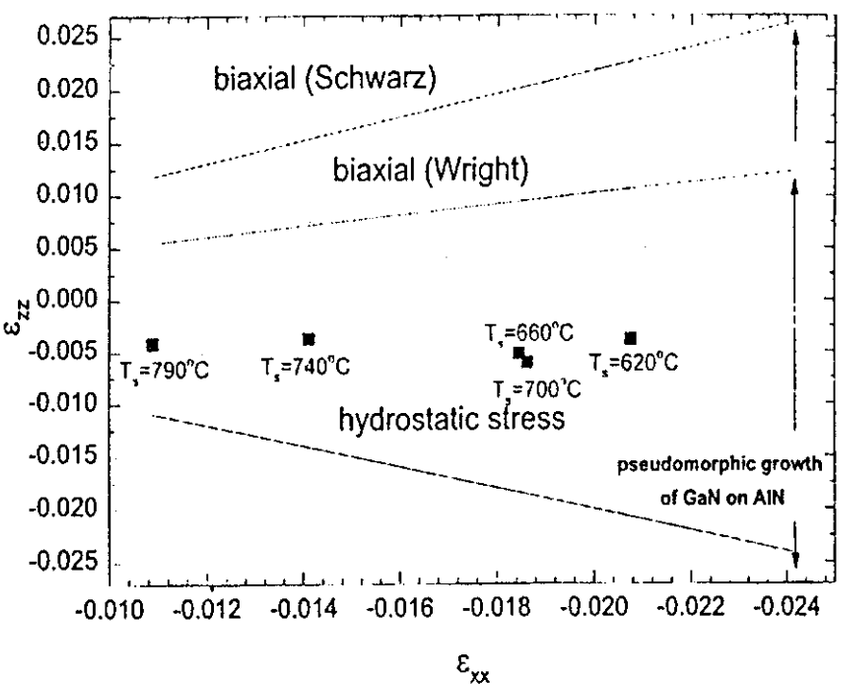
Two sets of samples were deposited by Molecular Beam Epitaxy with an RF plasma source for the activated nitrogen supply at the ISI, Forschungszentrum Jülich, Germany. The first set was deposited at a fixed substrate temperature of 790 °C with thicknesses between 2 and 6 nm; the second set consisted of equal thicknesses of 6 nm deposited at temperatures between 620 °C and 790 °C . AFM measurements were performed in order to probe the epilayer morphology and core level XPS provided a measurement of the polarization fields in the GaN [2].

X-ray absorption measurements were performed at the Ga K edge using a 7 element Ge hyper-pure Ge detector; polarization dependence of the XAFS signal was studied by orienting the sample either parallel or perpendicular to the growth plane. In all cases the local structure around Ga resembled that of bulk GaN, with no evidence of Ga-Al intermixing even at the lowest thicknesses; this testifies to the correctness of the growth procedures employed and to the high quality of the samples.

Analysis of the polarization dependent signals provided the in-plane and out-of-plane Ga-Ga second shell distances, which are simply related to the *a* and *c* lattice parameters of the wurzite structure. From the values of the lattice parameter the in-plane and out-of-plane strain values ε_{xx} and ε_{zz} were deduced.

The most interesting results were obtained from the temperature dependent series and they are reported in the figure where we plot values ε_{xx} and ε_{zz} as a function of substrate temperature. The lines correspond to theoretical predictions of either hydrostatic stress or biaxial stress for a 2D layer using the elastic constants published by two groups. In no cases were the experimental values of the strain found compatible with a pseudomorphic growth of GaN on AlN. However, as the substrate temperature is lowered the parallel strain approaches the values expected for pseudomorphic growth.

The above findings are qualitatively compatible with the AFM images which show that for all coverages the epilayer is composed of islands; with decreasing substrate temperature the average size of the islands decreases yielding a smoother epilayer. It is well known that in an island the distribution of strain is inhomogeneous, compressive near the base and tensile near the top; since XAFS measures an average strain state it is expected to measure smaller values of strain than for a flat 2D pseudomorphic growth. The decrease of the roughness with deposition temperatures is thus compatible with the increasing values of ε_{xx}. These results provide valuable insight in the growth mechanism of Nitrides which is useful for the understanding of the properties of heterostructures.



[1] F. Boscherini, R. Lantier, A. Rizzi, F. D'Acapito, and S. Mobilio, "Evidence for relaxed and high quality growth of GaN on SiC(0001)", Appl. Phys. Lett. **74**, 3308 (1999).

[2] A. Rizzi, R. Lantier, D. Freundt, F. Monti, H. Lüth, A. DiCarlo, F. DellaSala, and P. Lugli, J. Vac. Sci. Technol. B **17**, 1674 (1999).