Report on the beam time for the project 26 01 739
(DUBBLE station BM26A at the ESRF)
"GaN quantum dots structural peculiarities depending on the preparation conditions"

Developments of techniques allowing the determination of spatial and electronic structural parameters on the surface or interfaces of materials will provide tools to control and check the fabrication of structures containing nanoclusters with discrete electronic spectra. The fabrication of such systems can be an important step in the pathway towards miniaturization and engineering for quantum computer systems [1].

The spectrum of states in the self-organizing nanoclusters may be largely influenced by the elastic deformation at the boundaries arising from a mismatch of the lattice parameters of the nanocluster and substrate. The EXAFS- experimental technique allows determination of parameters regarding the local environment of atoms and electronic parameters of nanoclusters. In particular, our previous experiments using GeK XAFS showed that Ge QDs are characterized by interatomic Ge-Ge distances of 2.41Å which is 0.04 Å less than in bulk Ge [2-3].

The spectra have been measured on GaN/AlN heterosystems which contain GaN two-dimensional layers or nanoclusters on AlN substrates. These samples have been produced using molecular beam epitaxy (MBE) on (0001) sapphire substrate. The sample 1 consist of 20 layers with each an effective thickness of 4 GaN monolayers, sample 2 consist of 15 layers with each an effective thickness of 5 GaN monolayers. These layers are separated by AlN layers with a thickness of about 100Å. The GaN monolayer thickness is equivalent to 2.5Å (on average). The samples 3-6 consist of 1 GaN layer with each an effective thickness from 2 to 5 GaN monolayers. These layers are covered by AlN protective layers with a thickness of about 100Å.

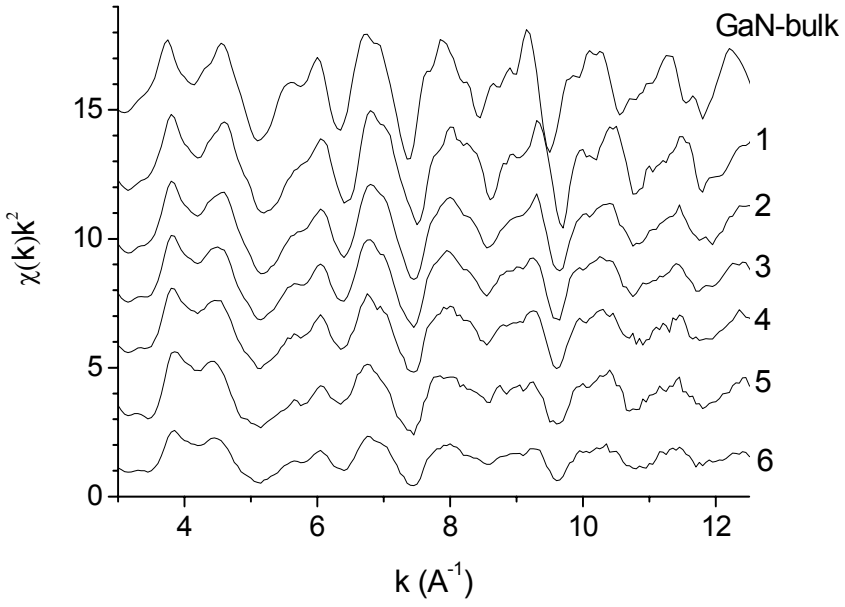

Figure 1. Experimental k^2-weighted Ga*K* EXAFS spectrum for bulk crystalline GaN and for GaN/AlN heterostructures.

As can be seen in the figure2, starting from the second coordination shell (2Ga), the peaks amplitudes for the GaN/AlN heterostructure are appreciably lower compared to these for the bulk GaN, indicating a decrease of Ga atoms in corresponding shells. This effect increased when moving from Sample 1 to Sample 6. All peaks corresponding to the higher shells exhibit some shape changes and shifts to lower distances. This is caused by some compression as a result the structural mismatch between the GaN clusters and the AlN substrate.

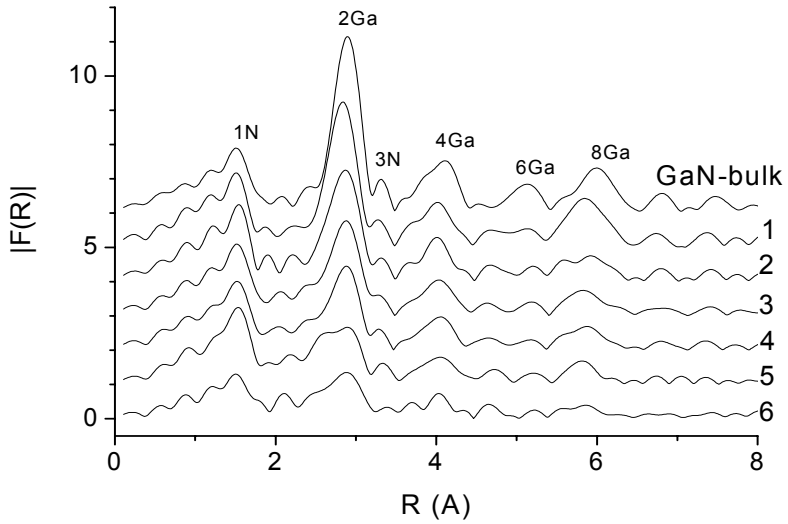

Figure 2. Fourier transform modules of $\chi(k)k^2$ GaK EXAFS without phase shift: for bulk crystalline GaN and for GaN/AlN heterostructures. The respective peaks are marked by the shell numbers and types of surrounding atoms in accordance with [4].

Table. Parameters of samples preparation ($T_{substrate}$ - temperature of AlN- substrate under GaN- deposition, ML number - effective thickness in monolayers of GaN film). Structure parameters of bulk GaN [4] and parameters obtained by fitting procedure for k^2-weighted Ga*K* EXAFS spectrum of bulk crystalline GaN and GaN/AlN heterostructures. R_1(Å), R_2(Å) – interatomic distances Ga-N and Ga-Ga, correspondingly; N_1, N_2 – coordination numbers of Ga by N and Ga by Ga; σ_1^2, σ_2^2 – Debye-Wallers factors (Å^2).

Sample	$T_{substr.}$ ºC	ML number	**R_1** ± 0.01Å **Ga-N**	**σ_1^2**±0.001Å^2 **Ga-N**	**N_1 Ga-N**	**R** ± 0.01Å **Ga-Ga**	**σ_2^2** ±0.001Å^2 **Ga-Ga**	**N_2** ± 0.3 **Ga-Ga**
GaN-bulk			1.95	0.007	4	3.18	0.006	12
1	600	4	1.93	0.005	4	3.13	0.006	10.7
2	400	5	1.93	0.004	4	3.15	0.006	8.7
3	400	5	1.94	0.004	4	3.16	0.006	7.4
4	400	3	1.94	0.005	4	3.16	0.005	5.9
5	500	2-3	1.94	0.004	4	3.15	0.005	6.2
6	400	5	1.97	0.015	3	3.15	0.006	4.1

Conclusion

It has been found that the first shell R_{Ga-N} interatomic distance in heterostructure GaN/AlN is equal to ~1.93 Å, which is 0.02 Å smaller compared to crystalline GaN. For the second Ga-Ga shell an interatomic distance R_{Ga-Ga} ~ 3.14 Å was found, which is 0.04 Å smaller than in crystalline GaN. The coordination number N_{Ga-Ga} was found to be from 5.9 to 10.7. It was established that heterostructure contains three-dimensional islands or two- dimensional thin films depending of temperature of AlN- substrate during GaN- deposition. Our results suggest that average size of GaN clusters and elastic strains and deformations depend of preparation conditions, such as temperature of AlN- substrate and time of deposition, or effective thickness of GaN film.

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References

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4. ICSD Collection Code 34476.