O-02

Ti INTERACTION WITH GaN SURFACE - A RESONANT PHOTOEMISSION STUDY

I.A. Kowalik[1], B.J. Kowalski[1], P. Kaczor[1], B.A. Orlowski[1], E. Lusakowska[1], R.L. Johnson[2], L. Houssian[3], J. Brison[3], I. Grzegory[4], and S. Porowski[4]

[1]*Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warsaw, Poland*
[2]*Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149, Hamburg, Germany*
[3]*University of Namur, FUNDP-LISE, Rue de Bruxelles 61, Namur, Belgium*
[4]*High Pressure Research Center, Polish Academy of Sciences, Sokołowska 29, Warsaw, Poland*

The detailed investigations of Ti/GaN contact formation are important for the sake of immediate practical applications. This system is attractive as an element of ohmic contacts in nitride-based electronic devices. It is also a suitable system for investigation of interactions between a transition metal and GaN surface. Ti/GaN system is a good example of reactive metal/semiconductor interface with interdiffusion of Ti into the substrate [1]. The resonant photoemission experiments was meant to show possible interactions between Ti atoms and clean GaN surface, to reveal compounds formed at the interface and to relate them to changes in the density of states distribution of the valence band of Ti/GaN system formed under ultra high vacuum conditions.

The bulk crystals of GaN were grown in the High Pressure Research Centre, Polish Academy of Sciences in Warsaw, Poland. The resonant photoemission experiments were performed at the Flipper II beamline (with monochromator operating in the photon energy range of 20-200 eV) at the HASYLAB synchrotron radiation laboratory in Hamburg, Germany. The GaN (000$\underline{1}$)-(1×1) surface was prepared *in situ* by repeated cycles of Ar^+ ion sputtering and annealing at 500°C under UHV conditions [2]. The surface crystallinity was assessed by low energy electron diffraction (LEED) method. Ti was deposited stepwise from a calibrated source.

The sets of photoelectron energy distribution curves were measured for clean GaN surface and as a function of Ti coverage (see Fig. 1). Ti deposition was begun with formation of a 2.7 Å thick layer. When the gradually increased thickness of Ti layer reached 6.75 Å, the sample was annealed in a few stages at 100-150°C. The changes in the electronic structure of the system, in the Ti 3*d* contribution, and the Ga 3*d* core-level were studied after each stage of Ti deposition and annealing. The experiments were performed for photon energies near to Ti 3*p*→3*d* excitation (46 eV). Thus, Ti 3*d* contribution to the emission from the valence band could be revealed due to its resonant enhancement. Interaction of Ti atoms with the GaN surface was also observed by spectroscopy of the Ga 3*d* core level. Acquired photoelectron energy distribution curves were complemented with spectra measured in the constant-initial-state mode, which clearly showed a Fano-type profile at the photon energy of about 46 eV (corresponding to Ti 3*p*→3*d* transition).

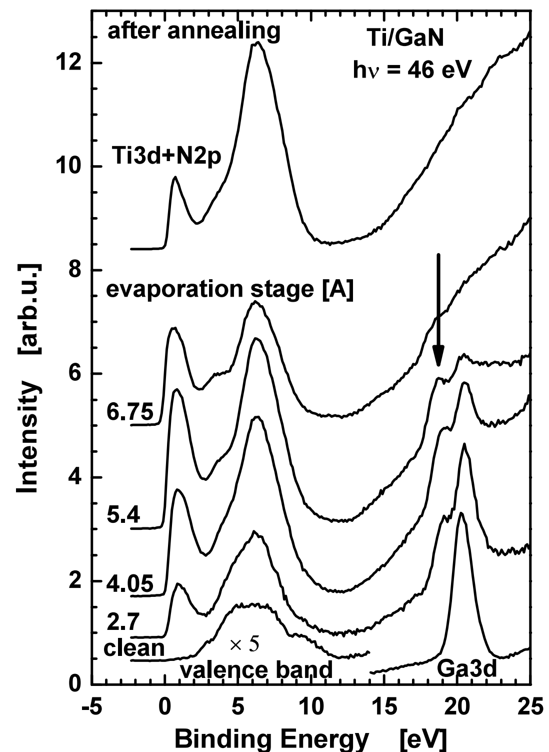

Figure 1. Selected photoemission energy-distribution curves obtained from GaN surface covered with Ti, measured for photon energy at the 3*p*→3*d* excitation.

The interface formation process deduced from the acquired data was proceeding in a few stages. First Ti deposition (about 2.7 Å) caused surface disruption, unbound Ga appeared on it (manifested in the feature marked by the arrow in Fig. 1). Further Ti deposition led to simultaneous formation of a Ti-N compound and increase of amount of metallic Ti covering the GaN surface and the Ga-containing-layer. Annealing process

enhanced reaction of Ti with N and the valence band became similar to that observed for titanium nitride [3]. Further evidence for presence of a Ti-N compound at the interface was obtained by SIMS - ToF measurements.

Morphology of the surface obtained by Ti deposition on GaN and annealing under UHV conditions was investigated *ex situ* by atomic force microscopy (AFM). The surface turned out to be atomically smooth with some, yet unidentified, terrace-like features of 5-20 nm height and lateral size up to 250 nm. The fragment of Ti/GaN surface is shown on the picture (Fig. 2).

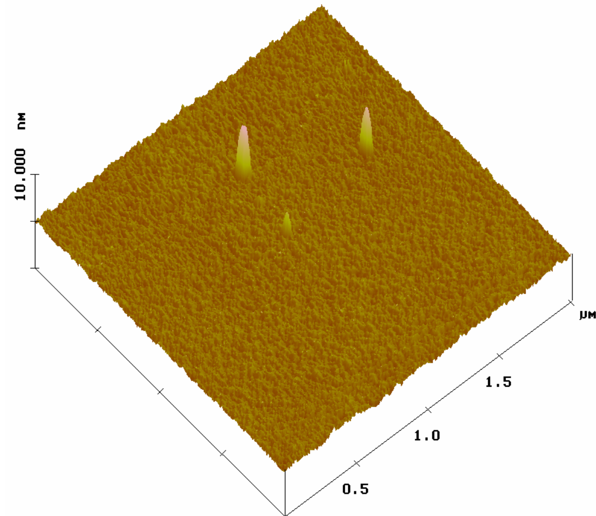

Figure 2. Surface morphology of 6.75 Å Ti deposited on GaN (000$\underline{1}$)-(1×1) and annealed under ultra high pressure conditions (obtained by AFM).

Acknowledgments This work was supported by KBN (Poland) project 2P03B 046 19 and by the IHP-Contract HPRI-CT-1999-00040/2001-00140 of the European Commission.

References

[1] J. Dumont, E. Monroy, E. Muñoz, R. Caudano, R. Sporken, *J. Cryst. Growth* **230** (2001) 558

[2] B.J. Kowalski, L. Plucinski, K. Kopalko, R. Iwanowski, B.A. Orlowski, R.L. Johnson, I. Grzegory, S. Porowski, *Surf. Sci*. **482-5** (2001) 740

[3] R.D. Bringans, H. Höchst, *Phys. Rev. B* **30** (1984) 5416

O-03

STUDIES OF Ge/Si NANOSTRUCTURES: PL, EXAFS AND TEM

I.N. Demchenko[1], K. Lawniczak-Jablonska[1], Z. Liliental-Weber[2], M. Chernyshova[1], E. Piskorska[1], M. Walczak[1], V. Glukhanuyk[1], D.N. Zakharov[2], M. Klepka[1], K.S. Zhuravlev[3], and E. Welter[4]

[1]*Institute of Physics Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668 Warsaw, Poland*
[2]*Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*
[3]*Institute of Semiconductor Physics, Siberian Branch of Russian Academy of Science, Lavrentieva 13, Novosibirsk, Russia*
[4]*HASYLAB at DESY, Notkestrasse 85, 22607 Hamburg, Germany*

Development of Si-based optoelectronics and the potential applications in microelectronics stimulate the interest in the physical properties of quantum confined semiconductor heterostructures. Therefore, these structures have attracted wide attention of scientific community, from both the experimental and the theoretical point of view.

The properties of Si/Ge/Si structures and Si/Ge superlattices were studied very actively by different methods. Nevertheless, there are still some questions concerning understanding and controlling of interface morphology in buried layers. Most of the investigated Si/Ge nanostructures have been prepared using conventional Stranski-Krastanov (SK) self-organized growth mode at high temperatures from 500 to 750ºC. In the presented studies the growth temperature of Ge layer was noticeably lower (from **210** to **250ºC**). This increases the possibility of Ge crystalline islands insertion into Si matrix without altering notably their shape and composition.

We will present the combined studies of 12ML and 20 ML of Ge buried in the silicon crystal (Si/12ML Ge/Si(001); Si/20ML Ge/Si(001)) and Si/(Si_mGe_n)×7/Si(001). To confirm the formation of quantum dots (QDs) in these samples, photoluminescence (PL) measurements were performed at 8 K using an Ar laser at a wavelength of 514.5 nm. The liquid nitrogen-cooled Ge detector was used for spectra collection. The dominant feature detected in the spectra is the luminescence band centered around 0.8 eV, which is commonly assigned to the Ge QDs photoluminescence.

It is known from the atomic force and electron microscopy that the QDs are formed above the critical thickness of Ge layer [4-6 monolayers (ML)]. At the first stage, perfect tetrahedral pyramids ("hut" – clusters) with side orientation of {105}-type are formed. There are no misfit dislocations in the "hut" – clusters, and the strain relaxation proceeds due to the partial elastic deformation. More relaxed QDs, with misfit dislocations are formed at the later stage of Ge film growth (>12 ML). The QDs have "dome" – clusters shape, with the main side orientation of {113}-type.

To check this observation at the more global scale and by non-destructive technique, quantitative and qualitative analysis of EXAFS data will be reported. The measurements were performed at HASYLAB A1 station at the angle of 45 degrees between incidence beam and sample surface. The analysis was done taking into account linear polarization of synchrotron radiation and with assumption of the solid solution of Ge_xSi_{1-x} inside QD. The existence of the interface between QD and Si matrix introduces a chemical disorder, which consequently increases the Debye-Waller factor value. The Artemis and Athena programs using IFEFFIT data analysis package were applied. The theoretical amplitudes and phases were calculated by FEFF8.

EXAFS analysis (Fig. 1 a, b) shows that in Si/Ge/Si structures grown by MBE at a low temperature 210 ºC (Ge layer) the QDs core consists of Ge atoms. There is some intermixing of Ge and Si atoms only at the surface of the Ge QDs. The small content of Si atoms provides an evidence that low growth temperature of Ge layers limits the silicon diffusion into quantum dots. For Si/12 ML Ge/Si(001), sample contraction of Ge-Ge bonds was observed in comparison with Ge-Ge bonds in Ge-crystalline material. These results suggest the presence of compressive strain in QDs. On the other hand the Ge-Ge bonds for the Si/20 ML Ge/Si(001) sample are found to be relaxed.

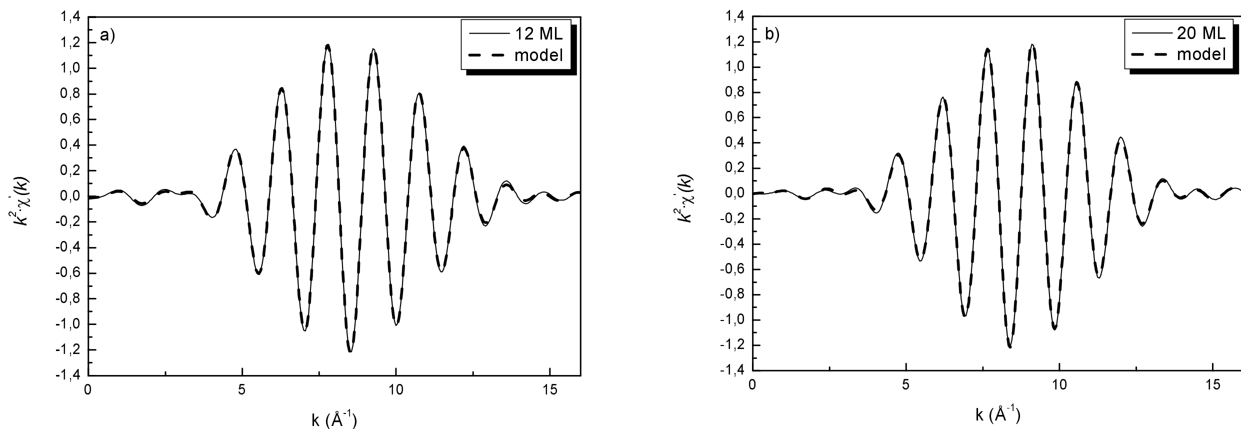

Figure 1. Least-squares fitting of the first coordination shell EXAFS oscillations (dashed line) and the experimental data (thin line) for: a) Si/12ML Ge/Si(001); b) Si/20ML Ge/Si(001) samples.

To confirm the results of EXAFS analysis the same samples were investigated by Transmission Electron Microscopy (TEM). The estimated sizes of QDs from cross-section and plan-view TEM studies agree with the sizes obtained from EXAFS analysis. In addition planar defects formed on {111} planes of the capping layer were also observed in cross-sectioned TEM samples. These defects start from the top of Ge layer [in the sample Si/12 ML Ge/Si(001)] and propagate to the sample surface. They are also visible on low magnification micrographs obtained under two beam conditions with $\vec{g}$ -vector $(\bar{1}1\bar{1})$ and $(02\bar{2})$. These defects were defined as stacking faults formed on {111} Si planes. With increase of Ge layer thickness (for the sample Si/20 ML Ge/Si(001)) the planar defects start to form at the base of QDs and propagate through the Ge layer to the sample surface. This confirms the suggestion of EXAFS analysis that with increase of Ge layer thickness from 12 ML to 20 ML the plastic relaxation of stress is taking place and dislocations are formed.

Acknowledgments: This work was partially supported by the State Committee for Scientific Research (Republic of Poland) (Grant No 2P03B05524 and 2P03B10625) and by the IHP-Contract HPRI-CT-2001-00140 and G1MA-CI-2002-4017 (CEPHEUS) of the European Commission. TEM part of work was supported by U.S. Department of Energy under the contract DE-AC03-76SF00098.