The Stillinger-Weber potential for AlN, GaN and InN

and atomic configuration of InGaN alloys

Huaping.LEI[1, 2], Jun.CHEN[1, 3], Sébastien.PETIT[1] and Gérard.NOUET[1]

[1] SIFCOM UMR 6176 CNRS-ENSICAEN , 6, Bd Marechal Juin, 14050 Caen, France

[2] Shanghai Institutes of Microsystem and Information Technology, CAS, Changning 865, 200050 Shanghai, China

[3]LRPMN, IUT Alençon, Université de Caen, 61250 Damigny, France

The Stillinger-Weber potentials for AlN, GaN and InN are modified in order to achieve a realistic description of the atomic configuration of InGaN and AlGaN alloys and their hetero-nanostructures. Firstly, for testing the validity of the SW potential parameters, the elastic constants of AlN, GaN and InN in the wurtzite and zinc-blende structures are calculated and most of them agree with the experimental or first-principle calculation values. In addition, the dependences of the atom energy on the volume per atom are presented for the three binary materials in the different crystal structures i.e. bcc, sodium chloride, wurtize and zinc-blende structure. The minimum of the atom energy in wurtzite and zinc-blende structures verifies they are more stable than the others. Based on the modified SW potential parameters, the distribution of indium atoms in InGaN alloys is studied. Three kinds of distribution are simulated: random, ordering and cluster. The results indicate that the atom energy is discrete regardless of In concentration. For the nitrogen atoms, five configurations with the different first-neighbors are found: N(4In) (-3.9eV), N(4Ga) (-4.5eV), N(2In,2Ga) (-4.23eV), N(3In,1Ga) (-4.05eV) and N(1In,3Ga) (-4.35eV) (Fig.1, indium atoms are randomly distributed in $In_{0.5}Ga_{0.5}N$ alloy). It can be inferred that the total energy of InGaN alloys without defects is approximately determined by the number of nitrogen atoms in the different configurations.

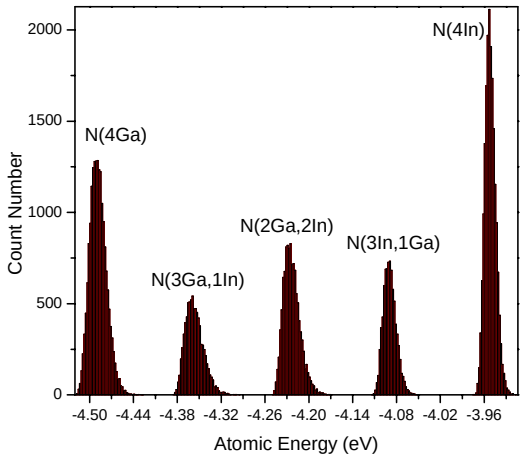

Fig.1: Atom energy for randomly indium atoms distribution in $In_{0.5}Ga_{0.5}N$ alloy.

In order to complete this SW potential approach, I plan to investigate nitride alloys within the framework of the density functional theory. As the number of atoms could be very large, we use the DFT program called AIMPRO which is particularly time-efficient. We consider the AlGaN and InGaN alloys. The work will include two parts:

1) The atomic structure and electronic bebaviour of ternary alloys with different compositions.

2) The microstructure of heterostructures including the defects and their electronic properties will be calculated and compared with the experimental results.