In epitaxial growth techniques such as Molecular Beam Epitaxy (MBE) or MOCVD, the properties of the growing material such stoichiometry, dopands and point defect concentrations, depends strongly on the surface thermodynamics and kinetics. Although both MBE and MOCVD are widely considered as highly non-equilibrium growth processes due to the large thermodynamic driving force, near thermodynamic equilibrium can be assumed near the gas-solid interface [1].

The bonding environment of the atoms in a surface layer differs from those of bulk atoms. The surface atoms will re-arrange themselves in order to reduce the surface energy. In general, structural reconstructions of semiconductor surfaces are driven and can be described by a few principles which include atomic relaxation, and electron counting rule. According to electron counting rule in heterpolar covalent or ionic semiconductors the electronic energy of the surface is lowered when charge is transferred from the cation dangling bonds (dbs) to the anion dbs. This is motivated by the fact that the anion dbs usually lye low in the bandgap.

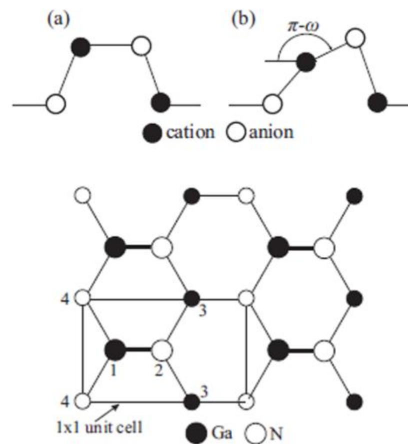

Figure 1: Side view of a III-V semiconductor (110) or (1$\underline{1}$00) surface, for (a) unrelaxed and (b) relaxed configuration.

Characteristic examples of ECR surfaces are the III-Nitride (1$\underline{1}$00) and (11$\underline{2}$0) non-polar and the (110) GaAs surfaces [2,3]. The surface relaxation of these surfaces is driven by electron-electron Coulomb repulsion, by quantum mechanical hybridization effects, and by classical Coulomb attraction between anions and cations. The aforementioned unrelaxed and unreconstructed surfaces consist of cation-anion dimers. Thus charge transfer from the energetically higher lying cation to the energetically lower anion db is taking place. Furthermore, in order to reduce the hybridization energy the cations tend to move below the surface and to establish planar sp^2-like bonds with their three nearest neighborhoods. On the other hand, the anions tend to move upwards and to establish a p^3-like configuration (see Fig. 1). The re-hybridization is forwarded by a rotation ω of the dimer. This rotation is accompanied by a lowering of the energy of the occupied anion dangling bond and by an increase of the energy of the cation empty state. Finally, the relevant cation-anion displacement costs electrostatic energy and in order to minimize it, the anion-cation distance tends to shorten. In this case the band structure of the corresponding surfaces is cleaned from any surface states (see Fig. 2).

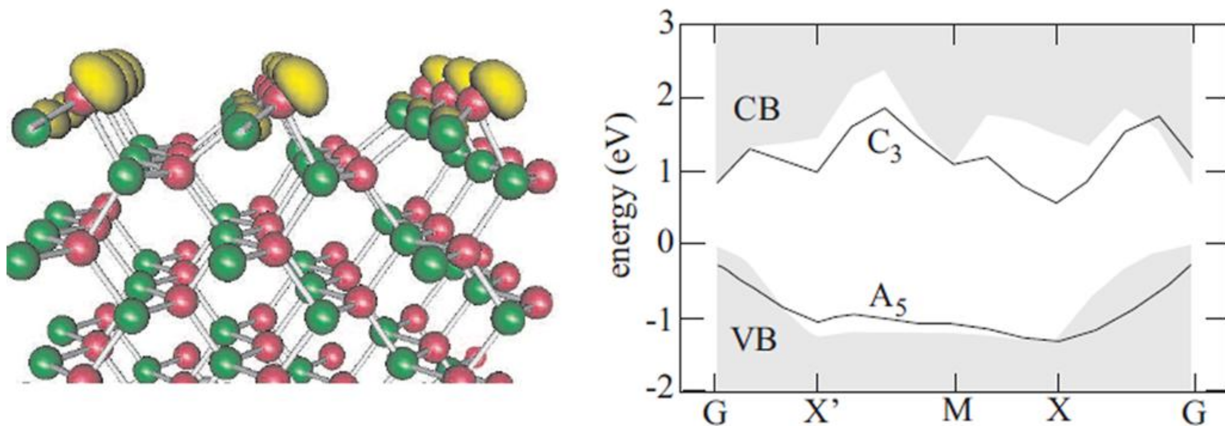

Figure 2: Right: Band structure for the GaAs(110) relaxed surface. The projected bulk band structures is indicated by the shaded areas. Left: Charge densities of the C3 and state at the M point of the surface Brillouin zone.

For polar and semipolar III-Nitride surfaces the aforementioned procedure results in surface periodicities (reconstructions) other than the 1x1. Characteristic examples are the 2x2 Ga adatom (0001) GaN and the *c*(2x2) AlAdatom (11$\underline{2}$2) AlN surfaces [4,5]. In both cases in order the surface to follow the aforementioned mechanisms has to reconstruct and expose a larger periodicity (see Fig. 3).

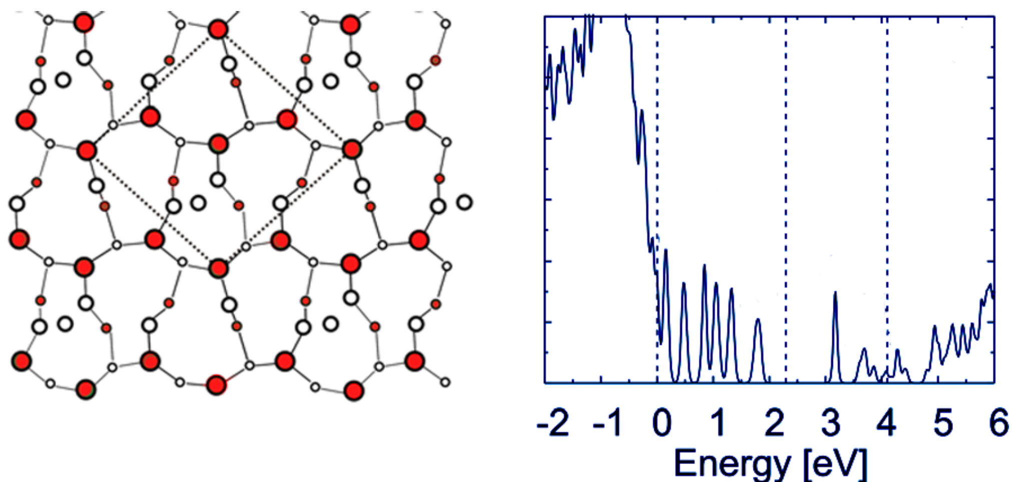

Figure 3: Left: Atomic geometry in top view of the c(2x2) Al adatom (11$\underline{2}$2) AlN surface. The dashed diamond indicates the c(2x2) cell. Red (open) balls indicate Al (N) atoms respectively. Righ: Density of states of the surface in the left. Left and right dashed indicate the VBM and CBM, respectively. The middle dashed lines indicates the position of the Fermi level. After Kalesaki et al., J. Appl. Phys. 112**, 033510 (2012).**

Apart from influencing the surface electronic structure and in turn the position of the Fermi level and the incorporation of dopands, surface reconstructions and morphologies have strong influence on the adatom kinetics. A peculiarity of the III-Nitride surfaces that has not be found for traditional III-V and II-VI semiconductors is that they stabilize excess metal in the form of single or multiple metal layers except for very N-rich conditions [6]. This has important consequences to the properties and the growth of these surfaces: Early works on GaAs or Si indicated that in order to achieve 2D step-flow growth mode

the growth temperature should be roughly half the melting temperature. However, for III-Nitrides growth these temperatures would require high Nitrogen overpressures which are not compatible with MBE [7]. Nevertheless, the tendency of III-Nitride surfaces to stabilize excess metal on the surface results in the self-surfactant effect [6] which substantially reduces the N adatom diffusion barriers, allows for efficient lateral surface transport and favors step-flow growth over three dimensional growth.

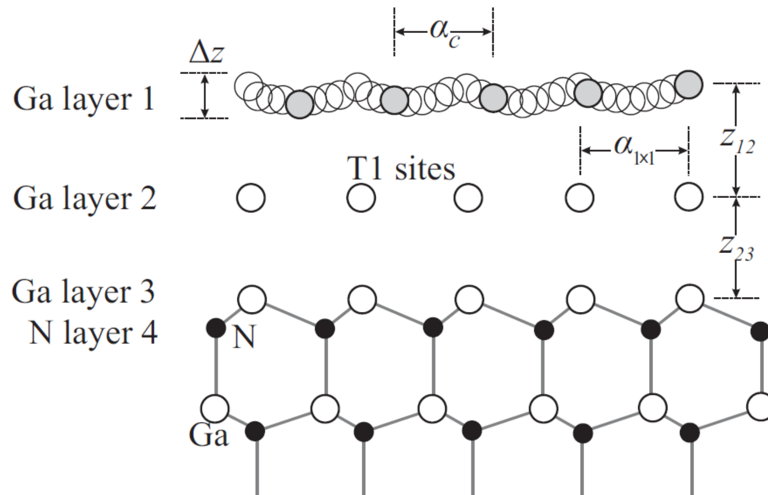

Figure 4: Side view of the $\sqrt{3}\times\sqrt{3}$ (0001) GaN laterally contracted Ga bilayer structure, proposed by Northrup *et al*. [8]. The filled circles in the top layer represent Ga atoms at a particular time. The open circles represent a time averaged image of the Ga atoms. The time averaged vertical corrugation of the top layer is approximately 0.16 Å.

A prerequisite to grow III-Nitride devices is to achieve a high control over the surface morphology during growth: In order to e.g. realize sharp heterointerfaces growth conditions that allows for 2D growth have to be identified. Ab initio based surface phase diagrams provide an on-atomic-scale description and understanding of the dependence of the surface morphologies on the experimentally relevant growth parameters such as partial pressures and temperatures. The general trends established so far for the growth of III-Nitride surfaces (i.e. ECR surfaces reconstructions for N-rich growth and metal rich surfaces for metal-rich conditions) offer the principles to explore and investigate the otherwise infinite pool of different surface geometries.

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