Role of electronic degrees of freedom in adsorption and the dynamics of the growth of semiconductor crystals and layers

Stanislaw Krukowski*, Pawel Strak, Pawel Kempisty
*lead presenter: stach@unipress.waw.pl
Institute of High Pressure Physics Polish Academy of Sciences, Sokolowska 29/37, 01-142 Warsaw, Poland

Semiconductor surfaces are haunted by large number of nonsaturated bonds that leads to considerable energy expense. The optimization of their energy leads to strong reconstruction processes showing the important role of electron degrees of freedom. Examples of such structures are presented and discussed. Energy optimization leads to severe consequences in adsorption of the atoms and molecules. Optimization processes does not change surface structure only, their occupation is also important. These processes sometimes induce drastic changes in the surface energy stabilizing specific structures, which was initially recognized as electron counting rule (ECR). It is shown that standard interpretation of ECR is oversimplification, nevertheless it is useful as standard ECR provides important guidance for selection of the most stable surface structures. It is proved that ECR states are characterized by the Fermi level free, i.e. not pinned by the surface states. That leads to direct relation between Fermi level in the bulk and the surface incorporation of the impurities as is investigated in the *ab initio* modelling of defect incorporation during growth. It is shown how full treatment of adsorption at semiconductor surface by incorporation of the entropy and other thermal effects changes the resulting surface diagrams. These data are expressed as the chemical potentials of the attached species that is translated into equilibrium partial pressures in the vapor. Full incorporation of these effect are facilitated be machine learning application for the *ab initio* data. These effects usually leads to drastically different growth conditions which affects surface diffusion and thermodynamic conditions at the steps.

References

[1] Krukowski S et al., Fermi level influence on the adsorption at semiconductor surface – ab initio simulations. J. Appl. Phys. 2013; 114:063507
[2] Strak P et al. Structural and electronic properties of AlN(0001) surface under partial N coverage as determined by ab initio approach. J Appl. Phys. 2015;118:095705.
[3] Kempisty P et al. Ab initio and thermodynamic picture of Al adsorption on AlN(0001) surface – role of bond creation and electron transition contributions. Appl. Surf. Sci. 2020;532:147719.
[4] Strak P et al. Adsoprtion of nitrogen at AlN(000-1) surface – decisve role of structural and electronic factors. Surf. Sci. 2021;713:121791.
[5] Strak P et al. Al coverage of AlN(0001) surface and Al vapor pressure – thermodynamic assessment based on ab initio calculations, Comp. Mater. Sci. 2022;203:111159.