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Lattice dynamics and thermodynamic stability of nitride semiconductors surfaces based on *ab initio* methods

Nowadays, scientists and engineers are expected to design and demonstrate more and more sophisticated devices. A large part of them is based on semiconductor materials, with III-nitrides among them. These semiconductors have already found a very wide application, among others, in optoelectronics as well as high-frequency and high-power devices. There is an opinion that the potential possibilities of these materials are still not fully explored, mainly due to the extremely difficult technology of their production, as well as due to insufficient knowledge of various phenomena. It is still advisable to perform basic research for these semiconductors. One of the key aspects is the knowledge of physics of phenomena occurring on the surface.

The subject of this project is the study of influence of temperature changes on the stability of III-N semiconductor (GaN, InN, and AlN) surface structures, starting from the basic laws of nature (*ab initio*), such as the laws of quantum mechanics and statistical physics. The problem to be resolved is the lack of agreement between the results obtained using the existing theoretical description in the literature and the results of observations and measurements, especially in the high temperature range. We have noticed that thermodynamic analysis available in the international literature often neglects the contribution from thermal vibrations of atoms and molecules on the surface, which may cause serious errors in the quantitative description. Our idea is to precisely determine the dynamic properties of the surface by first principles calculations and including the results in the thermodynamic description of nitride semiconductors surfaces. The most important and time-consuming task carried out in this project will be calculations based on the Density Functional Theory (DFT). Their results will allow us to reproduce the phonons spectra (quanta of vibration energy of crystal lattices) for systems representing surfaces. On their basis, we will be able to determine the missing contribution related to thermal changes of the condensed phase. This will enable performing a thermodynamic analysis with much greater accuracy than in previous studies. In this sense, the work planned in this project should be a step from a qualitatively consistent description towards a quantitatively consistent one.

The obtained results can be used in theoretical models of growth of nitride semiconductors, in particular regarding epitaxy from gas phase. The improvement of the theoretical description will allow a better control of crystallization process. Precise knowledge of surface conditions can provide the ability to incorporate specific dopants or change the concentration of unintentional impurities. A good knowledge of surface physics can significantly help in overcoming further technological barriers in the growth of nitrides crystals, layers, structures, and devices.