Growth and doping of semiconductors in vapor phase processes - ab initio analysis

1. Research project objectives/ Research hypothesis

The purpose of the research project " *Growth and doping of semiconductors in vapor phase processes - ab initio analysis* " is to formulate and verify the new hypothesis on the nature of the growth of semiconductor crystals and layers to obtain molecular level picture of growth, doping and surfactant effects during vapor growth processes. The basis of the formulation will be recently discovered charge transfer contribution to adsorption energy of the species at various semiconductor surfaces. The energy change related to transfer of electrons may reach several electronvolts with the magnitude of the effect depending on Fermi level. Growth proceeds in narrow adsorbate composition window, corresponding to electron counting rule (ECR). Thus extensive ab initio simulations employing large slabs will be used to elucidate problem of the relation of Fermi level, doping and surfactant role in the growth. The dynamic aspect of the charge transfer related issue is its participation in termalization after adsorption, i.e. the conversion of kinetic energy of adsorbed molecule to thermal energy of crystal lattice vibrations. The hypothesis is that the termalization occurs due to strong deviation of the system from Born-Oppenheimer approximation during fast adsorbate-surface collision. The process may play crucial role in the kinetic to thermal energy conversion. That stabilizes the adsorbate at the surfaces, the process important to incorporation of the dopants during growth. Altogether, the project will formulate molecular picture of the growth, doping and surfactant effects which is absent in present day state of art in the domain.

2. Basic research to be carried out

The following tasks will be realized

1. Determination of the structure of quantum states on selected basic clean surfaces of semiconductors .

2. Determination of the energetically stable configurations of molecules, radicals and atoms on the semiconductor surfaced, including dopants .

3. Determination of the quantum states related to adsorption of selected molecules on semiconductor surfaces , including molecular and dissociative adsorption.

4. Application of extended electron counting rule - (EECR) for determination of the areas with the defined position of Fermi level.

5. Intensive investigations of adsorption to verify EECR predictions. Determination of principal processes related to charge transfer from and to the surface.

6. Determination of thermodynamic dependences for the systems investigated within the project.

3. Expected impact of the project on the development of science, civilization and society

The obtained results will determine the dependence of the growth velocity and dopant incorporation on electronic properties of the surfaces and the crystal bulk. This indicates that in the case of Fermi level pinned surfaces the dependence on the pinning states emerges. That influences the adsorption, crystal and layer growth and incorporation of dopants.

The atomistic level picture of semiconductor growth is missing. The only proposed explanations assume difference between bulk properties, thus the surface factor is neglected, and therefore these models do not have predictive power. This is expected as the approach neglecting surface processes does not entail main issues of the growth of crystals.

The proposed explanation is the first model describing the doping processes during growth and epitaxy of semiconductors. These processes constitute the basis of the information technologies of present day civilization. Therefore the formulation of the proposed model will have possible influence on development of the future technologies.