Concept of Virtual Fabrication of Nanodimensional Semiconductor Heterostructures

Context. **Epitaxial growth methods** constitute a fundamental experimental technique of the modern technology of electronic materials fabrication. This technique supplies a possibility to obtain atomically thin epitaxial layers for the use in ultrathin-film device development and for production of epitaxial wafers for further development of integrated circuits consisting of monolayer-level controlled devices. **In this project this approach is extended to development of** a similar **3-dimensional (3D) processing in confined geometries,** such as nanopores of porous solids with thin pore walls. By manipulations of pore atomic surface structure, composition and topology, nanofluid composition, structure and chemistry, and process parameters it is expected to fabricate spatial nano-layered heterostructures that could be used as prototypes for 3D-integrated circuits of desired functionality. **The project is focused on development of a tractable and practical concept of virtual fabrication of nanodimensional semiconductor heterostructures (NHSs) at the atomic level** by processing of interfacial "fluids" composed of Ga, As, Al and P atoms in nanopore confinements of porous silicon structures**. The principal aims of the project include** (i) development of a tractable theoretical concept of 3D nanofluid processing in confinement based on the use and further generalization of the Pozhar-Gubbins theory of transport phenomena in nanosystems merged with the Hartree-Fock method and/or the density functional theory of the ground state; (ii) on the basis of the developed theoretical concept, prediction of the properties of the nanofabricated 3D NHSs at the atomic/molecular level in terms of the structure, composition and chemistry of the processed nanosystems and parameters of the processing methods; (iii) on the basis of this novel theoretical concept, development of simplified and practical engineering models of the "intelligent" nanosystems processing techniques that ensure desirable properties of the grown 3D NHSs (low/high band width, anisotropy of electron/hole transport, charge transport coefficients, etc.); (iv) development of theory-based, molecular simulations algorithms and codes to model the nanosystem processing that would allow to manipulate the grown NHSs properties by changing the processed nanofluid and the confinement lattice structure, composition, chemistry and process parameters; (v) on the basis of the developed models and software, development of a methodology for application of these engineering models to virtual nanofabrication of model 3D NHSs.

Objectives of this project development include:

- (i) to estimate fundamental constraints as applied to NHS processing in confined geometries; (ii) to generalise further and to merge the Pozhar-Gubbins theory of nanosystems with the Hartree-Fock and density functional theories of the ground state, with the objective to develop a unified theoretical description of the 3D NHS growth in confined geometries; (iii) to use this unified description to reveal correlations between structure, chemistry and composition of the nanofluid-confinement system and process parameters on one hand, and the band gaps, electronic charge densities, electron-phonon spectra, electron transports and interconnect conductance, etc., on the other hand;
- (i) to simplify the developed theoretical description, to formulate algorithms and to develop simulations models and software of the 3D NHS growth; (ii) to test the developed models by applying them to virtual fabrication of samples of GaAs/AlGaAs- and AlP-based NHSs carried by porous Si lattices; (iii) to compare properties of the virtually fabricated NHSs with those of existing similar heterostructures fabricated experimentally and evaluate performance of the developed models of the 3D NHS growth.

Significance and originality. Recent revolutionary progress in fabrication and characterization of electronic materials of the characteristic size of several hundred nanometers has already opened a new page in electronic device development. In this project we take further important step in this direction bringing the scale to several nanometers and investigating prospects of the "proper nanoscale" 3D processing of NHSs of desired electronic properties. This signifies an entirely new conceptual approach to electronic device (in particular high density integrated circuitry) design and technology, where functionality and hardware integration requirements are satisfied at the stage of the development of the nanoscale NHS materials. We believe that our attempt to develop a concept of virtual fabrication of 3D NHSs is the first attempt (i) to rationalize relations between the structure, composition and processing conditions of the 3D grown NHSs and their electronic transport properties, and (ii) to supply a unified theoretical and software support for the conceptual nanotechnological revolution.

Method. To study correlations between processed fluid properties and process parameters, the lattice structure, composition and chemistry, and the electronic properties of the emerging NHSs we plan to use theoretical methods of quantum statistical mechanics and statistical physics, and molecular simulations of the NHS grows. The standard Pozhar-Gubbins (PG) theory will be used to relate transport properties (diffusion and mobility) of the nanofluids processed in confinements and the process parameters. The PG functional perturbation theory (FPT) will be further generalized and used to describe non-equilibrium electronic phenomena (including charge transport) in emerging NHSs in terms of their ground state quantum correlators. Actual computations of these correlators will be performed using the Hartree-Fock and the density functional theory – based software as applied to the 3D NHSs recovered by the Car-Parrinello EMD simulations method. These data will be used in PG theoretical formulae to calculate electron and hole transport, interconnect conductance, etc. These theoretical predictions will be further evaluated against the results of the generalized Car-Parrinello NEMD simulation method as applied to the studied NHSs subject to the time independent external electrical fields. All these developments will supply a theory-based concept of manipulation of the nanosystem structure by changing the processed nanofluid and lattice composition/doping, chemistry, topology, and process parameters so that to ensure desirable band gaps, electronic charge densities, electron-phonon spectra, desired charge transport properties and interconnect conductance of the fabricated 3D NHSs.