Virtual Synthesis of 3D Nanoheterostructure Units With Pre-Designed Opto-Electronic Properties

INTRODUCTION

Recent sub-micron technologies for fabrication of nanoheterostructures (NHSs) used in electronic devices and integrated circuit manufacturing were facilitated by development of sophisticated nanoscale experimental techniques, such as scanning near field optical microscopy (SNOM or NSOM), improved epitaxial growth procedures (molecular beam epitaxy, or MBE, Stranski-Krastanow methods, and modified chemical processing), etc. These techniques led to fabrication of single semiconductor quantum dots (QDs) composed of Ga, As, Al, P, In, Sb, etc. atoms (where up to several thousand electrons are confined to a spatial region from tens to hundreds of nanometers in linear dimensions), as well as two-dimensional (2D) and three-dimensional (3D) ordered arrays of QDs that can act as NHSs. This project takes a further important step in this direction by bringing the scale down to tens of Angstroms, investigating the prospects of prediction of electronic properties from the first principles, and modeling the synthesis of 1 to 10nm-sized, 3D NHS units with designed electronic properties. Conceptually, this project approaches the problem from a functionality and hardware integration requirements point of view ("functions come first"-concept), rather than via a conventional route, where experimental fabrication of a NHS is attempted in advance of a reliable evaluation of its expected electronic properties.

There is a very low probability of this project to fail. This is because the methods that will be established in the course of this work are built from the first principles via further development and use of proven fundamental theoretical concepts, and computational and simulation techniques by an expert in the field, also possessing necessary computational equipment and tools.

AIMS AND OBJECTIVES

The ultimate goal of this project is to develop a self-consistent theoretical and computational concept and methods of virtual synthesis of electronic nanomaterials. Critical tasks of this project fall under two major thrusts as detailed below.

- **Theoretical developments:**
  - (i) Estimate fundamental constraints as applied to the simplest nanosystems in the confined geometries that can be used as "building blocks", or units, of NHSs;
  - (ii) Develop a novel, unified, projection-operator based, quantum statistical mechanical approach to nonequilibrium phenomena in nanosystems, and link this approach to the Hartree-Fock and DFT – based computations of the equilibrium state, to facilitate tractable description of quantum effects (such as quantum coherence and role of quantum confinement) and their impact on basic electronic properties (the electron level structure and existence of bands, charge transport coefficients, etc.) of 3D NHS units;
  - (iii) Use this unified description to reveal correlations between structure, chemistry and composition of the processed nanosystems and processing parameters on the one hand, and the band gaps, electronic charge densities, electron-phonon spectra, charge transport, etc. of the synthesized NHSs, on the other.
- **Development of a virtual nanofabrication methodology and its demonstration:**
  - (i) Simplify the developed theoretical approach to formulate algorithms and to develop computation and simulation models for virtual fabrication of the simplest prototype 3D NHS units via virtual nanoscale processing;
  - (ii) Implement the proposed models to "fabricate" virtual prototypes of GaAs, InAs and GaSb - based NHS units of designed conductance formed in nanopores of a porous silicate material;
  - (iii) Evaluate the developed theoretical and computational models via comparison of the theoretical/computational predictions of the tensorial conductivity in the studied NHS units and available experimental data;

(iv) Identify approaches and methods for future non-equilibrium simulations of the charge transport process that may be used as one of possible means to evaluate performance of the virtual synthesis methodology.

TIMELINESS, NOVELTY, AND SIGNIFICANCE

The aims of the proposed project coincide with at least four overarching goals of the NSF efforts to advance fundamental sciences and their applications (in particular, to nanomaterials synthesis). Specifically, the proposed project (1) *develops a fundamental scientific understanding of nanoscale phenomena*, such as synthesis and properties of electronic nanomaterials; is targeted at provision of (2) *the ability to design and synthesize materials at the atomic level to produce materials with designed properties and functions, including nanoscale assemblies*; focuses on (3) *attaining a fundamental understanding of the structural and dynamic aspects of nanoassemblies*, and provides for (4) *development of theory/modeling/simulation tools necessary to understand, predict, and control nanoscale phenomena*.

Fundamental and engineering sciences supply a rational foundation for novel technologies to support a strong economic growth of modern technology-based society. The development time for scientific concepts and methods to mature into technology ranges from 10 to 15 years. Therefore, now is high time to invest in conceptually new theoretical/computational tools necessary to advance further nanomaterials technologies. In the course of the proposed project such tools will be developed and applied to manipulate synthesis of advanced materials at the atomic scale, and to provide such models of the synthesis that would permit manipulation of synthesized electronic nanomaterials properties. This project is the first step undertaken to advance a novel concept of virtual synthesis of materials via development of a unified (theoretical, computational and simulation), self-consistent, fundamental and tractable approach to facilitate nanofabrication of 3D NHS units by design. The project will use and develop further novel theoretical, computational and simulation methods and techniques described below in detail. In addition, this project realizes an extraordinary opportunity for a female, minority theoretical scientist to contribute significantly to existing methods enabling yet another technological revolution.