Appendix A

Statement of Work

Proposal Number UTDW 00024

Prepared by Sandia National Laboratories

"Physical & Chemical Sciences Designated Capabilities"

I. Description of Services

PROJECT SCOPE:

Overview:

We propose to undertake work in the three task areas of diagnostics and characterization, synthesis and processing, and theory and simulation. These areas span the fields of semiconductor physics, electronic materials, nanostructures, surface physics and chemistry, plasma and chemical processing, lasers and optics, pattern recognition, remote sensing, ion-solid interactions and radiation effects physics, and advanced materials sciences. The tools we will use to address these areas also span a wide range of disciplines ranging from first principles modeling and atomic scale measurement to remote laser sensing and new approaches to pattern recognition. Many of these tools are unique, either individually or in combination, and hence are of benefit to industrial and university partners with needs in research, development and/or production in related areas of technology.

TECHNICAL CONTENT:

Work to be performed will fall into one or more of the following three Task Areas:

Task 1 — Diagnostics and Characterization

We will apply our unique combination of diagnostic and characterization tools to solve research, development, and production problems. Our tools are particularly well suited to situations where higher resolution (spatial or spectroscopic) or an integrated understanding enabled by the use of multiple tools is required. The technical features include:

— **Sandia Tandem Van de Graaff Ion Accelerator Nuclear Microprobe**
Sandia will provide energy >4 MeV, nuclear microscopy and radiation effects microscopy. This 6 MV tandem accelerator generates ion species from hydrogen to bismuth for both radiation effects research and quantitative ion beam analysis of materials containing light elements (hydrogen to fluorine) using heavy ion elastic recoil detection (ERD) and heavy elements using high-energy back scattering spectrometry. An external Micro Ion Beam Analysis (X-MIBA) capability enables multi-elemental analysis and ion irradiation of samples, which are vacuum incompatible or extraordinarily large. The Sandia Nuclear Microprobe with micrometer size high-energy ion beams is used to study materials and devices. Special emphasis is given to the evaluation of the radiation hardness of microelectronic devices using three new advanced diagnostic techniques invented at Sandia: Single-Event-Upset Imaging, Ion-Beamed-Induced-Charge Collection Imaging (IBICC), and time-resolved IBICC.

— **Vision-Science Laboratory**
The vision science laboratory consists of state-of-the-art hardware and software capabilities for carrying out video inspection, multi-spectral image analysis, and sensor-based pattern recognition. (Includes Imaging Processing System, Patent #5,495,536). These capabilities are used in applications ranging from microsensor-based chemical detection and recognition to automated video/SEM inspection of semiconductor materials and circuits. (Patent #5,901,247) This is a new approach to pattern recognition, coupling perception-oriented research with machine algorithms.

— **Chemical Vapor Deposition (CVD)**
Sandia will provide experimental tools for investigating CVD which include optical probes (such as reflectance-difference spectroscopy) for gas phase and surface processes, a range of surface analytic techniques, molecular beam methods for gas/surface kinetics, and flow visualization techniques. These tools are also integrated in a unique manner with research CVD reactors and with advanced chemistry and fluid models.

— **Growth Science Laboratory**
Sandia has capabilities for in-situ characterization of materials during thin film deposition, molecular beam epitaxial growth, and low energy ion beam simulated growth, using intensity profile sensitive reflection high energy electron diffraction (RHEDD) for surface structure, energy dispersive x-ray reflectometry for in-situ surface and interface structure, multibeam wafer curvature for strain (Patent #5,912,738), and Auger electron spectroscopy for surface composition.

— **KMAP X-ray Diffractometer**
Based on double crystal x-ray diffractometry in combination with position sensitive x-ray detection our KMAP x-ray diffraction analysis is used to determine the lattice constant, strain relaxation, composition, layer orientation, and mosaic spread of a large variety of advanced epitaxial semiconductor materials.

— **Atomic-Level Imaging and Spectroscopy**
We have developed unique capabilities in:

- Atomic Force Microscopy (AFM) with molecular resolution, temperature control, and simultaneous fluorescence detection.
- Scanning Tunneling Microscopy (STM) in terms of ability to track single atoms
- Low Energy Electron Microscopy (LEEM) in terms of spatial resolution and spectroscopic imaging capability
- Field Ion Microscopy (FIM) in terms of single atom resolution and accurate temperature control to 1 Kelvin
- Interfacial Force Microscopy (IFM) with feedback for accurate force profile measurements
- Near Field Scanning Optical Microscopy (NSOM) for sub-diffraction limited optical imaging with combined shear force feedback and IFM

— **Nanoelectronics Laboratory**
Sandia has capabilities for fabrication of nanoscale quantum device structures together with capabilities for ultra-low noise measurement of transpsort form 0.3 Kelvin to ambient at high magnetic fields.

— **Lasers and Optics**
Sandia will provide characterization and advancement of the understanding in the area of solid-state lasers and non-linear optics, especially as coherent sources of broadly tunable light in rugged, compact geometries. We have established expertise in long-term and transient radiation effects characterization of optical materials. (Includes patented Wavefront Sensor Patent #5,493,391, and Monolithic Optical Amplification Devices Patent #5,463,649). Sandia has capabilities in combined modeling and laboratory validation for non-linear materials as well as in rad-characterization (pulsed nuclear reactor, and X-ray generators).

— **Laser and Optical Spectroscopies**
Sandia has capabilities in characterizing semiconductor materials by photoluminescence and magnetoluminescence down to low temperatures by optical laser imaging and laser microscopy, by laser excitation spectroscopy, and by the time-resolved measurements of optical emission. We also have developed a high lateral resolution, near-field scanning optical microscopy (NSOM) capability with time and frequency resolution.

— **Low Temperature Plasma Analysis**
We have state-of-the-art capabilities for the analysis of low-temperature plasmas as found in commercial processing reactors. These include emission spectroscopy, electrical characterization, laser and microwave-based measurements of species concentrations, in situ electric field measurements and others. Sandia is the only lab, which combines new diagnostics, relevant process chemistries (complex mixtures), and massively parallel (MP) computer models for simulation of continuous and transient plasmas.

Task 2 — Synthesis and Processing

We will apply our facilities and personnel expertise for synthesis and processing of novel materials requiring higher accuracies, or greater understanding of the link between process and performance, than normal. These facilities and expertise range from chemical processes such as chemical vapor deposition to physical processes such as pulsed laser deposition to complex multi-phenomena processs such as ECR plasma deposition and etching. Our technical capabilities include:

— **Nanocluster Laboratory**
We have developed and patented a process based on the use of inverse micelles for the synthesis of large quantities of monodisperse clusters of metals, semiconductors, and oxides.

— **Electron Cyclotron Resonance (ECR)**
This plasma facility has been built for studying fundamental processes governing the growth of oxide and nitride dielectric films used in optoelectronics and used as hard coatings. This is the only system in the U. S., that combines ECR plus e-beam evaporation.

— **Molecular Beam Epitaxy**
We have research semiconductor growth laboratories for ultra-pure and ultra-flexible MBE growth of III-V materials. In addition, we have research systems for beam-enhanced Group IV semiconductor growth.

— **Metal-Organic Chemical Vapor Deposition (MOCVD)**
We maintain research facilities with capabilities in MOCVD of compound semiconductor materials. These capabilities include research reactors designed specifically for studies of CVD chemistry, fluid dynamics, the development of advanced in-situ diagnostics, and the development of advanced semiconductor heterostructures.

— **Crystal and Thin Film Growth**
Capabilities in this area include a pulsed laser deposition chamber, a thin film oxide deposition chamber, a diamond-like carbon deposition chamber, a hot filament, chemical vapor deposition chamber, and various apparatus for single crystal growth. Our capabilities for stress relief of diamond-like carbon films and structures produced by pulsed laser deposition are not available elsewhere.

Task 3 — Theory and Simulation

Our capabilities in theory and simulation can be applied toward understanding of the synthesis and properties of new materials and/or structures. They are particularly valuable for understanding how to tailor or tune properties for specific applications. The technical capabilities include:

— **Chemical Processes**
We have extensive capabilities, including massively parallel computation, to model complex chemically reacting flows such as occur in chemical vapor deposition manufacturing processes. Our numerical simulations can include the coupled gas-phase and gas-surface chemistry, fluid dynamics, heat, and mass transfer to provide predictive models of a chemical process.

— **Low-Temperature Plasmas**
We have extensive capabilities in massively parallel codes to simulate the time and space evolution of low-temperature plasmas, focusing on new theoretical techniques for achieving rapid convergence and on direct comparisons with experimental results.

— **Electronic Structure and Linear Scaling**
We have developed state-of-the-art massively parallel electronic structure algorithms, based on ab initio pseudopotentials and plane-wave/Gaussian basis functions. These codes are used to develop a fundamental understanding of physical phenomena and materials, including compound semiconductor band structure, diffusion of point defects, dopants and impurities, optoelectronic properties of extended defects, adsorbate interactions on surfaces, bonding at metal-oxide interfaces, and enhanced reactivity of nanoparticles. To allow the investigation of more complex systems and phenomena, we have developed new computationally efficient algorithms, e.g., self-consistent linear scaling density functional theory, and variable and real-space gridding.

II. Deliverables:

The deliverables will consist of reports summarizing work performed and associated results. It is possible that samples developed will also constitute a deliverable depending on customer requests.

This project and the work being proposed are unclassified.