Statement of Work

Umbrella Technical Description of Work (UTDW0024)
"Physical, Chemical and Nano Sciences Designated Capabilities"

Updated April 2006

Sandia National Laboratories, for and in consideration of the funding provided by the Sponsor, shall perform the following work for the Sponsor:

I. Description of Services

PROJECT SCOPE:

<u>Overview</u>:

We propose to undertake work in three task areas: (1) diagnostics and characterization, (2) synthesis and processing, and (3) 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:

— **Atomic-Level Imaging and Spectroscopy**
We have developed unique capabilities in:
- Scanning Tunneling Microscopy (STM) with the ability to track the diffusion of single atoms on surfaces,
- Low Energy Electron Microscopy (LEEM) with nanometer spatial resolution and real-time spectroscopic imaging capability at sample temperatures from 300K to over 1000K
- Field Ion Microscopy (FIM) with single atom resolution and accurate temperature control to 1 Kelvin,
- Atom Probe Microscopy (APM) with pulsed laser desorption capability,
- Interfacial Force Microscopy (IFM) with feedback for accurate, simultaneous normal and frictional force profile measurements for the quantitative study of adhesion, tribology, and nanomechanics, and
- Atomic force microscopy (AFM) for imaging, force profiling, and manipulation of individual biomolecules in fluid environments with simultaneous fluorescence detection.
- Piezo Force Microscopy (PFM) for measuring piezoelectric coefficient, imaging ferroelectric domains, and spatial variation in piezoelectric properties, and input.

— **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.

— **Electrochemical Scanning Probe Microscopy**
We have developed the ability to study nanoscale changes at surfaces during oxidation and dissolution of metal surfaces under electrochemical control using scanning tunneling microscopy. These studies can be performed in a variety of electrolytes in order to determine the mechanisms governing passive film growth.

— **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, 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.

— **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 gold 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 submicrometer 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. We have also developed the Ion Electron Emission Microscope (U. S. Patent No. 6,291,823 and 2001 R&D-100 Award winner), which can perform radiation microscopy using very highly ionizing particles without focusing the ion beam. A recent extension of this microscope is a desktop version that uses an alpha radiation source, called the Ion Photon Emission Microscope (which also received an R&D 100 Award in 2005).

— **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.

— **Laser and Optical Spectroscopies**
Sandia has capabilities in characterizing semiconductor materials by photoluminescence and magneto-luminescence 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.

— **Lasers and Optics**
We provide characterization and advanced 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 also have established expertise in long-term and transient radiation effects characterization of optical materials. Capabilities include the widely used (approximately 2000 users worldwide) SNLO (Sandia Non-Linear Optics) code, which is a lab-tested code for predicting the performance of non-linear optical components. In the area of integrated optical materials, our laboratories produce new types of photosensitive materials (processing patent applied for) for directly-writeable waveguides and reconfigurable optical interconnects.

— **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.

— **Materials Microcharacterization**
Our capabilities in this area include optical microscopy, scanning, electron microscopy, analytical transmission electron microscopy, double crystal x-ray diffraction, ion beam analysis of materials (RBS, channeling, ERD, PIXE, NRA), Hall measurements, microcalorimetry, photoluminescence, light scattering, electronic transport, deep level spectroscopy, magnetization, and dielectric and magnetic susceptibilities.

— **MEMS-based Tensile Testing**
We have developed the capability to perform pure uni-axial loading of metal MEMBS test structure in situ and ex situ of a TEM. The technique has been demonstrated using Al, Ni and Cu, but is applicable to a wide range of other materials.

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

— **Scanning Cathodoluminescence Microscopy**
We have developed the ability to measure and image cathodoluminescence from insulators and semiconductors on the submicron scale in order to understand how defects influence the emission of light from the ultraviolet to the visible. Individual spectra are also obtained at controlled locations in order to identify heterogeneities.

— **Scanning Probe Metrology**
We have developed a unique wide-field scanning Interfacial Force Microscope with calibrated force detection for the dynamic measurement of normal and lateral forces of micro-electrical-mechanical system components in operation.

— **Simultaneous Measurement of H, D, and T in Materials**
We have designed and implemented a new ion beam analysis (IBA) system to simultaneously measure the absolute quantities of H, D, and T in materials using an elastic recoil detection (ERD) technique. The technique uses an E-dE detector arrangement, or particle telescope, to provide for accurate separation of the H, D, and T signals. The system can also simultaneously acquire information about medium and high Z elements in the sample using Rutherford backscattering spectrometry (RBS). Measurement of other light elements is possible using the nuclear reaction analysis (NRA) technique, which is isotope specific. The system will have an accuracy of $< 2\%$ for measuring the composition of solids.

— **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.

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 processes such as ECR plasma deposition and etching. Our technical capabilities include:

— **400 keV and 180 keV Ion Implanters**
These systems are equipped with a variety of sources (gas, sputter, and metal vapor). This facility provides ion species from hydrogen to bismuth that can be used for studying fundamental irradiation mechanisms and selective chemical doping in semiconductors, metals, ferroelectrics and superconductors. The 180 keV Implanter is capable of both ambient and high temperature implants up to 600°C and ion currents up to 50 micro-A.

— **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.

— **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.

— **High Pressure and Shock Wave Physics and Chemistry Laboratories**
Our capabilities in this area include large volume static high pressure apparatus which can be operated at temperatures ranging from 2 to 700 K and in magnetic fields, as well as gas gun and explosive loading facilities with state-of-the-art, time-resolved diagnostics. Recovery fixtures have been developed for use with the gas gun and explosive shock loading facilities that allow unique material synthesis over broad ranges of shock pressures and temperatures.

— **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.

— **Molecular Beam Epitaxy (MBE)**
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.

— **Nanocluster Laboratory**
We have developed numerous processes for the synthesis of large quantities of monodisperse particles and clusters of metals, semiconductors, and oxides.

— **Soft Nanolithography**
Soft nanolithography refers to patterning techniques that complement UV and electron beam lithography. These approaches avoid the chemical and radiation exposure often used in conventional lithography processing, making soft nanolithography particularly useful for bio, organic, and molecular materials. Current capabilities include micro-contact printing, nano-transfer printing, and dip-pen nanolithography.

— **Stress Evolution During Electrodeposition**
We have developed the capability to measure stress evolution during thin film electrodeposition and have used it to measure stress during patterned and unpatterned film growth. Our studies range from fundamental mechanisms that create stress during island coalescence to materials-specific systems, such as electrodeposited Ni, Cu, Sn, Ag and their alloys.

— **Synthetic Organic Laboratory**
Novel lipids, surfactants, and other small molecules are prepared in this laboratory via synthetic organic techniques. The laboratory is also capable of forming and characterizing self-organized structures (e.g., liposomes, micelles, self-assembled monolayers, LB films) generated with the newly synthesized molecules in pure or mixed molecular systems.

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 that 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.

— **Complex System Analysis**
We have developed a suite of tools to manage complex data collections and process them to produce user defined information. One key advantage of our approach is that the user employs high-level interactions to process the data and is freed from traditional programming language constructs.

— **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.

— **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.

— **Molecular Dynamics Simulation**
Large scale, classical molecular dynamics simulations using the massively-parallel code LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) are being used to model a wide variety of systems. These classical simulations cover the length and time scale intermediate between quantum and continuum calculations. Systems of current interest include adhesion and friction in self-assembled monolayers, degradation of polymer adhesives, wetting and spreading of multi-component fluids and transport in polymer membranes for fuel cells. Modifications of the algorithm to include particle rotation and friction have been implemented to study granular materials.

— **Optical and Wave Propagation**
We have developed advanced simulation codes for understanding wave propagation in optical parametric oscillators and amplifiers for the purpose of designing highly efficient, tunable laser sources. We also have capabilities in novel optical designs, including resonators for compact laser geometries. These capabilities are coupled to in-house micro-optics construction facilities and state-of-the-art optics testing.

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.