**LaboratoryName: Idaho National Laboratory**
**B&R Code: KC 0202010**

**FWP and possible subtask under FWP:**
Structural and Electrostatic Effects in Interface and Nanostructure Growth
**FWP Number: 3E106(100390)**
**Program Scope:** The goal of this work is to explore some of the ways that non-idealities in solids, such as interfaces, surfaces and defects, affect their materials properties of relevance to the DOE missions. Specifically, it explores (1) the dynamics of compound formation at metal/semiconductor interfaces, including the formation of metastable compounds; (2) the role of surface bonding in determining nanoparticle binding energies, and hence their melting, sublimation and sintering behaviors; and (3) the effect of substitutional defects on the properties of layered superconductors.

**Major Program Achievements (over duration of support):**
The most tangible achievements to date are the following publications:
1) H. H. Farrell, C. D. Van Siclen, D. M. Ginosar, L. M. Petkovic, and R. D. Parra, "Surface Bonding Effects in Nanoparticles: Stoichiometric Compound Semiconductors " submitted to *J. Vac. Sci. Technol.B.*
2) H. H. Farrell and C. D. Van Siclen, "Binding Energy, Vapor Pressure, and Melting Point of Semiconductor Nanoparticles", *J. Vac. Sci. Technol.B.* **25**, 1441 (2007).
3) H. H. Farrell and R. A. LaViolette, "Diatomic Substitutionals in Superconducting $Nb_{(1-x)}B_2$", *Physica C-Superconductivity and Its Applications*, **449** 1 (2006).
4) H. H. Farrell, J. L. Hilton, B. D. Schultz BD, C. J. Palmstrøm, "Nonequilibrium Phases in Epitaxial Mn/GaAs Interfacial Reactions" *J. Vac Sci. Technol.* B **24**, 2018 (2006).
5) H. H. Farrell, A. B. Denison, "Semi-empirical inelastic mean free paths for positrons", *Surface and Interface Analysis*, **37**, 529 (2005).
6) H. H. Farrell and R. A. LaViolette, "Anion Variations at Semiconductor Interfaces: ZnSe(100)/GaAs(100), *J. Vac. Sci. Technol. B,* **23**, 406 (2005).
Publications in preparation include:
7) Sergey N. Rashkeev, Daniel M. Ginosar , Lucia M. Petkovic , and Helen H. Farrell, "Catalytic Activity of Supported Metal Particles for Sulfuric Acid Decomposition Reaction", in preparation.
8) H. H. Farrell and R. D. Parra, "Binding Energy of Oxide Particles", to be submitted to *J. Phys. Chem. B.*
9) R. D. Parra and H. H. Farrell, "Copper Oxide Clusters", to be submitted to the *J. Chem. Phys.*
10) H. H. Farrell, "Binding Energies of Compound Semiconductor Nanoparticles", to be submitted to *J. Vac. Sci. Technol.B.*
11) H. H. Farrell and Randall A. LaViolette, "The McMillan Equation as Applied to Metal Diborides", to be resubmitted to Phys. Rev. Lett.
Papers 2, 4 and 6 have also been given as talks at the '05, '06, and '07 annual PCSI meetings, respectively. An extension of paper 6 was also given at the 2005 MRS meeting and paper 1was given at the 2007 AVS meeting. An invited talk entitled "Computational Modeling of Nanostructures" was given at the NSF sponsored workshop "United States-Ireland Partnership Nanotechnology Workshop", Belfast, Northern Ireland, October 23rd and 24th, 2006.

**Program impact:**
Work progresses on understanding the relationship between the forces that govern the formation of defects, surface and interfaces, and their effects on the relevant materials properties.
**Interactions:** Idaho National Laboratory; C. D. Van Siclen, D. M. Ginosar, L. M. Petkovic, S. Rashkeev. Sandia National Laboratory; R. A. LaViolette (formerly INL).
University of Minnesota at Minneapolis; C. J. Palmstrom. DePaul University; R. D. Parra.
Pennsylvania State University; Darrell Schlom,
**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):** Laboratory Director's Award for Individual Lifetime Achievement in Science and Technology. Program Committee: Physics and Chemistry of Semiconductor Surfaces Annual Meetings.
**Personnel Commitments for FY2007 to Nearest +/- 10%:**
Helen H. Farrell, 50 %.
**Authorized Budget (BA) for FY05, FY06, FY07:**
**FY02 BA $200K** **FY03 BA $200K** **FY04 BA $200K**