COMPUTATIONAL NANOENGINEERING LABORATORY

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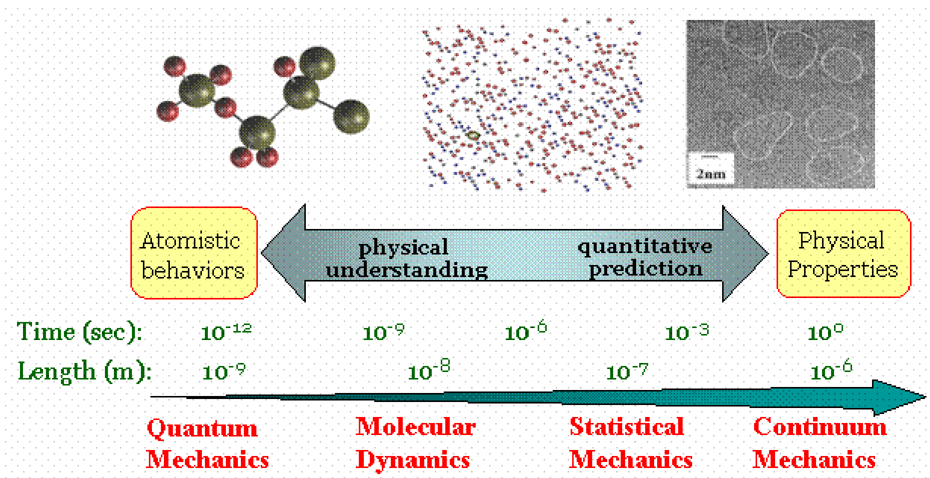
A. DESCRIPTION OF RESEARCH INTERESTS AND MOTIVATION:

Research in my group has a well-balanced emphasis on fundamentals and applications, ranging from first principles studies of surface chemistry, bulk dynamics, and interfacial interactions to multiscale, multiphysics modeling for manufacturing and fabrication of novel electronic, chemical, and biological devices.

Our research interests lie in developing (1) strategies for predictive multiscale, multiphysics computational models which can be utilized to guide the rational design and fabrication of future nanoscale devices and (2) a detailed understanding of the relationship between synthesis, structure, and properties of nanostructured materials and systems.



Why computational nanoengineering?

The ability to control the structure and function of matter at the nanometer scale offers enormous opportunities to create new materials and components with unique and valuable properties --- leading to the burgeoning interest in nanotechnology. A nanometer is one billionth of a meter, or just three to four atoms wide. As a reference point, the average human hair is about 25,000 nanometers wide. Red blood cells have an average diameter of approximately 8000 nm. Below 100 nanometers in size, the properties of materials are mainly governed by the laws of quantum mechanics, rather than classical Newtonian physics, and thus depend strongly on their size and shape. The ultimate goal of nanotechnology, perhaps, is to develop novel nanodevices for various applications in electronics, sensing, catalysis, and other fields, based upon complete control of creating and integrating diverse functional materials, components and systems at the nanoscale from 1 to 100 nanometers.

Since carbon nanotubes were first discovered in 1991, researchers have successfully synthesized and characterized a variety of nanostructured materials and components. In most cases, however little is known about how synthesis conditions of tiny materials influence their structure and properties. A critical issue for further advances in nanotechnology is to gain a deeper understanding of quantitative relationships between the synthesis conditions, structure and properties. Experiments may yield many clues to the behavior of nanomaterials, but their interpretation is often controversial due largely to difficulties in direct measurements. To explore the complex synthesis-structure-property relationships, the Hwang group has used multiscale computational approach which seamlessly combines various state-of-the-art theoretical methods that range from quantum chemistry, molecular mechanics, to statistical and continuum-level theories.

Recent advances in computational quantum mechanics with significantly increased computing power allow first principles prediction of atomic-level interactions in various materials systems. However, the inherent physical length and time scales required for describing growth, diffusion and phase transformation in nanoscale materials and systems are far beyond the current capability of first principles quantum mechanics. Systematic integration of first principles descriptions into larger scale simulations based on statistical and continuum models is therefore necessary to develop robust computational tools that allow accurate prediction of the unusual behavior and properties of materials at the nanoscale.

My group has been active in developing strategies for multiscale modeling of the synthesis and manipulation of inorganic nanostructures and the connection between their synthesis, structure and properties, for various applications ranging from nanoscale electronic devices, portable fuel cells, to chemical and biological sensors. Included among his current research interests are:

- Examination of how silicon nanocrystals form in a silicon-rich oxide matrix, and effects of process conditions on the nanocrystals size and shape, and subsequent charge retention and optical properties. The embedded nanocrystals system is a leading contender for use in furthering the miniaturization of silicon devices far below 100 nanometers. Potential applications include: non-volatile computer memory devices which are widely used in digital cameras and mobile phones; and chip-to-chip optical interconnects which will replace current copper-based wiring technology when copper traces no longer can keep up with future generations of smaller, smarter and faster computers; and
- Exploration of how the preparation and operation conditions of various metal alloy nanocatalysts influence their size, shape and composition, and subsequent catalytic activity. The theoretical efforts assist greatly in designing and synthesizing new high performance nanocatalysts based on less expensive non-precious metals, reducing the high cost of catalysts caused by current exclusive use of platinum in fuel cell applications.

In addition, a significant portion of the Hwang group research concern: atomic-level control of the surface chemistry and electrical properties of silicon and oxide nanomaterials through impurity doping as well as strain and defect engineering; and electrochemical and plasma-assisted nanopatterning of semiconductor and metal surfaces.

The interdisciplinary research program provides an ideal training ground for students interested in the newly emerging field of computational nanotechnology.

B. CURRENT AND FORMER GROUP MEMBERS:

We have openings for one or two PhD students.

Current Members:

- **Eight (8)** Ph.D Students
- **One (1)** Visiting Professor

Former Members:

- Taras Kirichenko (PhD, 05/2005, Freescale Semiconductor, Inc., Austin, Texas)
- Decai Yu (PhD, 01/2006, Spansion, Inc., Sunnyvale, California)
- Scott Harrison (PhD, 05/2006, Spansion, Inc., Sunnyvale, California)
- Devina Pillay (PhD, 08/2006, NRC Postdoctoral Fellow, Naval Research Laboratory)
- Jason Kenney (PhD, 01/2007, Applied Materials, Inc., Santa Clara, California)
- Yun Wang (Postdoc, 2002-2004, Associate Professor, Shanghai Jiao Tong University)
- Chin-Lung Kuo (Postdoc, 2005-2007, Assistant Professor, National Taiwan University)

C. AWARDS AND HONORS TO STUDENTS:

- Invited Participant in the East Asia and Pacific Summer Institutes Program (Stephens) 2008
- DohWonSuk Memorial Award (Lee) 2007
- Applied Materials Graduate Fellowship (Paek) 2007
- CCG Excellent Award, The American Chemical Society (Pillay) 2005
- F. M. Becket Summer Fellowship, The Electrochemical Society (Harrison) 2005
- University Continuing Fellowship, UT-Austin (Pillay) 2004
- Invited Participant in the East Asia and Pacific Summer Institutes Program (Kenney) 2004
- University Continuing Fellowship, UT-Austin (Harrison) 2004
- Travel Grant, Electronics Division, The Electrochemical Society (Harrison) 2004
- Invited participant in a Pan-American Advanced Studies Institute program (Kenney) 2003

D. PUBLICATIONS AND PATENTS/DISCLOSURES FROM THE HWANG GROUP

Patents/Disclosures

1. "Method for Predicting the Synthesis, Structure and Properties of Si Nanocrystals Embedded in Oxide Matrices," with D. Yu, US Patent --- *Commercialized!*

2. "First-principles Model for Predicting the Evolution of N-type Dopant Concentration and Electrical Activity Profiles in Ultrashallow Junction Formation," with S. Harrison, US Patent --- *Commercialized!*

Invited Book Chapters

1. J. Kenney and **G.S. Hwang**, "Basics: Handling Techniques – Etching," The Encyclopedia of Electrochemical Power Sources, Elsevier, in press (2007).

Peer Reviewed Journal Articles

76. C.-L. Kuo and **G.S. Hwang**[#], "Strain-induced Formation of Surface Defects in Amorphous Silica: A Theoretical Prediction," *Phys. Rev. Lett*. **100**, 76104 (2008).

75. J.A. Kenney, E. Paek, and **G.S. Hwang**, "Stochastic Plasma Charging of Nanopatterned Dielectric Surfaces," *IEEE Trans. Plasma Sci., Special Issue: Images in Plasma Science*, in press (2008).

74. C.-L. Kuo and **G.S. Hwang**, "On the Origin of Nitrogen-induced Retardation of Boron Diffusion in Amorphous Silica," *Appl. Phys. Lett*., in press (2008).

73. S. Lee and **G.S. Hwang**, "Structure and stability of small compact self-interstitial clusters in crystalline silicon," *Phys. Rev*. B, in press (2008).

72. S.H. Lee and **G.S. Hwang**, "Structure, energetics and bonding of amorphous Au-Si alloys," *J. Chem. Phys* **127**, 224710 (2007).

71. D. Yu, S. Lee, and **G.S. Hwang**, "On the Origin of Si Nanocrystal Formation in a Si Suboxide Matrix," *J. Appl. Phys.* **102**, 84309 (2007).

70. J. Shin, H.-W. Kim, **G.S. Hwang,** J.G. Ekerdt, "Chemical routes to ultra thin films for copper barriers and liners," *Surface & Coatings Technol.* **201**, 9256 (2007).

69. S. Harrison, T. Edgar, and **G.S. Hwang**, "Prediction of B-Si_i-F Complex Formation and Its Role in B TED Suppression and Deactivation," *J. Appl. Phys.* **101**, 66102 (2007).

68. J. Kenney and **G.S. Hwang**, "Prediction of stochastic behavior in differential charging of nanopatterned dielectric surfaces during plasma processing," *J. Appl. Phys.* **101**, 44307 (2007).

67. J. Shin, A. Waheed, W.A. Winkenwerder, H.-W. Kim, K. Agapiou, R.A. Jones, **G.S. Hwang,** J.G. Ekerdt, "Chemical Vapor Deposition of Amorphous Ruthenium-Phosphorus Alloy Films," *Thin Solid Films.* **515**(13), 5298 (2007).

66. C. Kuo and **G.S. Hwang**, "Structure and Interconversion of Oxygen Vacancy Related Defects on Amorphous Silica," *Phys. Rev. Lett.* **97**, 66101 (2006).

65. D. Pillay, Y. Wang, and **G.S. Hwang**, "Prediction of Tetraoxygen Formation on Rutile TiO_2(110)," *J. Am. Chem. Soc.* **128**, 14000 (2006).

64. J. Shin, A. Waheed, K. Agapiou, W.A. Winkenwerder, H.-W. Kim, R.A. Jones, **G.S. Hwang**, J.G. Ekerdt, "Growth of Ultra-thin Films of Amorphous Ruthenium-Phosphorus Alloys Using a Single Source CVD Precursor," *J. Am. Chem. Soc.* **128**, 16510 (2006).

63. S. Harrison, T. Edgar, and **G.S. Hwang**, "Prediction of Anomalous Fluorine-Silicon Interstitial Pair Diffusion in Crystalline Silicon," *Phys. Rev. B-rapid communication* **74**, 121201 (2006).

62. S. Harrison, T. Edgar, and **G.S. Hwang**, "Interstitial-Mediated Mechanisms of Arsenic and Phosphorus Diffusion in Silicon," *Phys. Rev. B* **74**, 195202 (2006).

61. S. Harrison, T. Edgar, and **G.S. Hwang**, "Interstitial Mediated Arsenic Clustering in Ultrashallow Junction Formation," *Electrochem. Solid-State Lett.* **9**, G354 (2006).

60. D. Pillay and **G.S. Hwang**, "O_2-Coverage Dependent CO Oxidation on Reduced TiO_2(110): A First Principles Study," *J. Chem. Phys.* **125**, 144706 (2006).

59. D. Pillay and **G.S. Hwang**, "Structure of Small Au_n, Ag_n, and Cu_n Clusters (n=2-4) on Rutile TiO_2(110): A Density Functional Theory Study," *J. Mol. Struct.-THEOCHEM* **771**, 129 (2006) (*invited contribution*).

58. J. Kenney and **G.S. Hwang**, "Computational Analysis of Intratool Interactions in Electrochemical Micromachining with Multitip Tool Electrodes," *Electrochem. Solid-State Lett.* **9**, D21 (2006).

57. J. Kenney and **G. S. Hwang**, "Etch trends in electrochemical machining with ultrashort voltage pulses: Prediction from theory and simulation," *Electrochem. Solid-State Lett.* **9**, D1 (2006).

56. S. Harrison, T. Edgar, and **G. S. Hwang**, "Structure, Stability, and Diffusion of Arsenic-Silicon Interstitial Pairs," *Appl. Phys. Lett.* **87**, 231905 (2005).

55. D. Yu, T.A. Kirichenko, S. Banerjee, and **G. S. Hwang**, "Structure and Diffusion of Excess Si Atoms in SiO_2," *Phys. Rev. B* 72, 205204 (2005).

54. L. Lin[#], T. Kirichenko, B. Sahu, **G. S. Hwang**, S. Banerjee, "Theoretical study of B diffusion with charged defects in strained Si," *Phys. Rev.* B **72**, 205206 (2005).

53. S. Harrison, T. Edgar, and **G. S. Hwang**, "Structure and Dynamics of the Diarsenic Complex in Crystalline Silicon," *Phys. Rev. B* **72**, 195414 (2005).

52. D. Pillay and **G. S. Hwang**, "Growth and Structure of Small Au particles on TiO_2(110) Rutile," *Phys. Rev. B* **72**, 205422 (2005).

51. T. Kirichenko, D. Yu, S. Banerjee, and **G. S. Hwang**, "Silicon interstitials at Si/SiO_2 interfaces: Density functional calculations," *Phys. Rev. B* **72**, 35345 (2005).

50. D. Pillay, Y. Wang, and **G. S. Hwang**, "Growth, Structure, and Chemistry of 1B Metal Clusters supported on TiO_2(110): Atomic Level Understanding from First Principles Studies," *Catalysis Today* **105**, 78 (2005). *(Invited contribution)*

49. J. Kenney and **G. S. Hwang**, "Electrochemical machining with ultrashort voltage pulses: modeling of charging dynamics and feature profile evolution," *Nanotechnology* **16**, S309 (2005). *(Invited contribution)*

48. Y. Wang and **G. S. Hwang**, "Origin of Non-local Interactions in Adsorption of Polar Molecules on Si(001)-2×1," *J. Chem. Phys.* **122**, 164706 (2005).

47. Y. Wang and **G. S. Hwang**, "P-Assisted Growth of Molecular Wires on Si(001)-2×1," *Appl. Phys. Lett.* **86**(2), 23108 (2005). (Selected for the January 17, 2005 issue of *Virtual Journal* of Nanoscale Science & Technology)

46. S. Harrison, T. Edgar, and **G. S. Hwang**, "Interaction between interstitials and arsenic-vacancy complexes in crystalline silicon," *Appl. Phys. Lett*, **85**(21), 4935 (2004).

45. L. Lin, T. Kirichenko, S. Banerjee, and **G. S. Hwang**, "Boron diffusion in strained Si: A first principles study," *J. Appl. Phys.* **96**(10), 5543 (2004).

44. T. Kirichenko, S. Banerjee[#], and **G. S. Hwang**, "Surface Chemistry Effects on Vacancy and Interstitial Annihilation on Si(001)," *Phys. Status Solidi B* **241**(10), 2303 (2004).

43. S. Harrison, T. Kirichenko, D. Yu, T. Edgar, S. Banerjee, and **G. S. Hwang**, "Origin of vacancy and interstitial stabilization at the amorphous-crystalline Si interface," *J. Appl. Phys.* **96**(4), 3334 (2004).

42. Y. Wang, D. Pillay and **G. S. Hwang**, "Dynamics of oxygen species on reduced TiO_2(110) rutile," *Phys. Rev. B*, **70**(4), 193410 (2004).

41. T. Kirichenko, S. Banerjee, and **G. S. Hwang**, "Interactions of neutral vacancies and interstitials with the Si(001) surface," *Phys. Rev. B* **70**(4), 45321 (2004).

40. J. Kenney, W. Shin and **G. S. Hwang**, "Two-dimensional Computational Model for Electrochemical Micromachining with Ultrashort Voltage Pulses," *Appl. Phys. Lett*. **84**(19), 3774 (2004).

39. Y. Wang, S. Lee and **G. S. Hwang**, "Effect of Subsurface Boron and Phosphorus on the Surface Reactivity of Si(001): Water and Ammonia Adsorption," *J. Phys. Chem. B* **108**, 16147 (2004).

38. T. Kirichenko, S. Banerjee, and **G. S. Hwang**, "Mechanisms of Monovacancy Annihilation and Type-A Defect Creation on Si(001)-2×1," *Surf. Sci.* **555**(1-3), 187 (2004).

37. D. Pillay, Y. Wang and **G. S. Hwang**, "A comparative theoretical study of Au, Ag and Cu adsorption on TiO_2(110) rutile surfaces," *KJChE* **21**(2), 537 (2004) *(invited contribution)***.**

36. Y. Wang and **G. S. Hwang**, "Two Dimensional Arrangement of CH_3NH_2 Adsorption on Si(001)-2×1," *Chem. Phys. Lett*. **385** (1-2), 144 (2004).

35. D. Pillay, B. Steward, C. Shin and **G. S. Hwang**, "Revisit to an Ising Model for Order-Disorder Phase Transition on Si(001)," *Surf. Sci*. **554** (2-3), 150 (2004).

34. Y. Wang and **G. S. Hwang**, "Function of Subsurface Boron on Si (100)-2×1: Water Adsorption," *Surf. Sci*. **547**, L882 (2003).

33. Y. Wang and **G. S. Hwang**, "Adsorption of Au atoms on stoichiometric and reduced TiO_2(110) rutile surfaces: a first principles study," *Surf. Sci*. **542** (1-2), 72 (2003).