

Final Technical Report on Project “Growth of Quantum Wires on Step-Bunched Substrates”, Grant Number: DE-FG03-01ER45875

PI: Feng Liu

Funding Period: June 2000 to May 2004

I. Accomplishments

We have had a very productive period during the funding cycle that began in June 2000 and ended in May 2004. We have published/submitted 34 papers and 28 of them include the acknowledgement to the support by Department of Energy. These include 12 in Physical Review Letters (submissions in review and in press not counted), 1 in Nature, and 7 invited review papers and book chapters. Our work has been featured in Nature Materials Highlights and in popular Science journals and magazines and in newspapers. Our work has won the 2002 DOE “Chucky Bullet” competition in Materials and Engineering Physics category and made into DOE Weekly (Research Highlights) 8 times. The PI has been selected as a member of the DOE reviewer panel for the Materials and Engineering Physics Research Program at the Sandia National Laboratory-NM. The PI has been invited to give 31 invited talks, including 15 at the national and international conferences/workshops and 16 seminars/colloquia at universities and research institutions/laboratories around the world. One student received Ph.D. and two received Masters degree under the PI’s supervision during this period. The PI has been supervising eight graduate students and two postdoctoral fellows and has hosted three visiting professors. In the following, we present in detail the highlights of research completed, the list of resulting publications, recognitions/honors/awards during the funding period, professional activities, including invited talks and organization of conferences, degree earned by students, personnel supported and research collaborations.

II. Research Highlights

We have had many exciting moments during the funding period, as reflected, for example, by our high-profile publications of 12 Physical Review Letters, 1 Nature and 7 invited reviews. To summarize our main research achievements and to give an overview what we have done, below I present the 8 Weekly (Research Highlights) we submitted to DOE during the funding period.

(1) Lattice Mismatch Leads to Devices: Devices are often made from materials with different atomic sizes. The strain due to lattice mismatch is a key factor in determining the materials properties and hence the device performance. In the past, scientists have mostly been concerned with lattice matching of different elements in the design and fabrication of devices. More recently, however, strain engineering, in particular the strain-induced self-assembly and self-organization, has been recognized as a unique method for fabricating nanostructures, such as quantum wires and quantum dots. In a series of three publications in the *Physical Review Letters*, Professor Feng Liu at the University of Utah and his collaborators have discovered several novel physical mechanisms for strain-induced self-organization of nanostructures. For example, in growth of two-dimensional islands (quantum disks), they demonstrated that strain not only induces a uniform island size, as has been shown previously, but also directs island

motion that leads to both uniform island size and uniform island spacing. Based on this mechanism, it is possible to fabricate a large ordered array of nanostructures with both uniform size and uniform spacing required for device applications.

(2) Self-Assembled Quantum Dots on Deformable Substrates: Properties of ultra-small nanostructures such as quantum dots are intrinsically linked to their immediate surroundings. Application of quantum dots in future devices requires a fundamental understanding of not only the properties of quantum dots themselves but also their interactions with the surroundings. However, most studies have focused only on the properties of nanostructures themselves. In a recent communication, published in *Nature*, Professor Feng Liu at the University of Utah and Professor Max Lagally at University of Wisconsin-Madison reported a novel growth morphology of self-assembled germanium (Ge) quantum dots on ultra-thin silicon (Si) deposited on insulator (SOI) substrates. The work describes an intriguing interplay among the growth of Ge dots, the localized bending of Si templates, and the viscous flow of the SiO₂ substrate. The Ge dots serve as a localized source of stress, causing the silicon template to bend beneath each Ge dot and hence a localized change of the band gap. Unique and unusual electronic, electrical, and optical properties are expected. These findings have significant implications on the use of SOI in the semiconductor industry because the localized stress in SOI becomes an increasingly significant issue as the size of device shrinks toward the nanometer scale.

(3) Novel Mechanism for Self-Organized Nanoscale Pattern Formation on Surface: Surface patterning is critical for electronic device fabrication, especially at the nanoscale where conventional lithographic techniques are not applicable. A new approach to surface patterning involves a self-organization process. The critical issue of self-organization is controlling the length scales. In a recent publication in *Physical Review Letters*, Professor Feng Liu at the University of Utah demonstrated the creation of identical nanoscale surface patterns with controllable length scales. He introduced a two-step model in which the first step defines the periodicity of the pattern and the second step controls the size of the pattern. The model quantitatively explains some unique patterns formed on the Silicon (111) surface, recently observed jointly by two experimental groups at Chung-Cheng University, Taiwan, and the University of Wisconsin-Madison. It provides a general scheme for creating well-ordered surface patterns to be used as templates for subsequent nanofabrication.

(4) Mechanism for Self-Assembly of Three-Dimensional Metal Islands in Heteroepitaxy: Nanotechnologies of the future will demand the creation of large arrays of nanostructures (e.g., quantum wires and dots) with uniform size and spacing. One approach to the creation of such arrays is to “let nature do it”, for example, by self-assembly of three-dimensional (3D) islands in heteroepitaxial growth. Remarkable size uniformity has been achieved for the growth of both 3D elemental and compound semiconductor islands. However, the size uniformity of 3D metal islands is less common and generally harder to achieve. In a recent publication in *Phys. Rev. Lett.*, Professor Feng Liu at the University of Utah has demonstrated a mechanism of growing uniform 3D metal islands. He introduced a new model for the growth of 3D metal islands on insulator substrates with an additional term of island edge energy. The existence of such

island edge effect makes the island shape dependent on island size and induces self-assembly of islands with uniform size. Therefore, it provides a general scheme of nanofabrication for creating uniform sized 3D metal islands.

(5) Stressful Ge islands reshape Si film: Mechanical properties of thin films play an important role in determining the performance, reliability, and lifetime of device. As the size of device continues to shrink toward the nanometer scale, the mechanical behavior of nanoscale thin films (or materials in general) is expected to be different from their bulk counterparts. However, a qualitative and/or quantitative assessment of such differences remains to be established for most systems. In a recent publication in *Phys. Rev. Lett.*, which made also to the September issue of Nature Materials Research Highlights, Professor Feng Liu at the University of Utah and Prof. Max Lagally at University of Wisconsin-Madison have demonstrated a unique nano-mechanical behavior of ultra-thin Si film occurring during growth of strained Ge islands on silicon on insulator (SOI) substrate. The stressful Ge islands reshape the Si film in a dramatic fashion, inducing an anomalous large and localized bending of Si film underneath the Ge islands. Molecular dynamics simulation shows that a transition from the normal extended thin film bending to such unusual localized bending occurs when local stress is applied to a film whose thickness is reduced to a few nanometers. Such transition is expected to occur generally in any solid thin film.

(6) Observing the 'Wings' of Atoms --- imaging atomic orbitals by atomic force microscope: An atom is made of a nuclear core surrounded by electrons, which move around the nucleus in atomic orbitals. Depending on the size of an atom, atomic orbitals adopt different geometries, pointing out in different directions like atomic 'wings'. The Nobel prize-winning invention of scanning tunneling microscope (STM), and its cousin atomic force microscope (AFM) has allowed us to see directly individual atoms on a solid surface. However, atoms generally appear as a single protrusion (blur) in the STM and AFM images because the microscope can't resolve the details of atomic orbitals. In a recent publication in *Phys. Rev. Lett.*, Professor Feng Liu at the University of Utah and his students have demonstrated, using extensive quantum-mechanical calculations, the feasibility of seeing not only the atom but also the atomic orbitals when imaging the surface with AFM. They show that the key condition for seeing the atomic wings is to bring the AFM tip so close to the surface (~1-2 angstroms) that the force between the tip atom and the surface atom becomes angular dependent, sensitive to the orientations of atomic wings.

(7) Computational Designing of Carbon Nanotube Electromechanical Device: By investigating the correlation between mechanical and electrical properties of carbon nanotubes using first-principles quantum transport calculations combined with structural simulations, Professor Feng Liu at the University of Utah and his colleagues have recently designed a series of nanoscale electromechanical devices, including pressure sensors, switches, and transistors. One example of their study has recently been published in *Phys. Rev. Lett.* When a material is mechanically deformed, its electrical property also changes. Such correlated effect becomes even more pronounced at the nanometer scale, and provides the bases for designing nanoscale electromechanical devices. Furthermore,

recent advances in computational algorithms and supercomputers have allowed accurate prediction of structural, mechanical and electrical properties of materials, which brings a new era of computational designing of novel nanoscale materials and devices.

(8) Guiding Quantum Dots on Curved Surface: Self-assembly of three-dimensional (3D) islands in heteroepitaxial growth has been recognized as a unique *natural* path for fabricating quantum dots (QDs). Remarkable size uniformity has been achieved for self-assembled QDs. However, their spatial ordering is usually poor because islands nucleate at random positions on surface. In a recent publication in *Phys. Rev. Lett.*,²² Professor Feng Liu at the University of Utah and Prof. Lagally at University of Wisconsin have proposed a new concept of guiding QDs on a curved surface by a local-strain-mediated control of surface chemical potential. They achieve ordered growth of compact 1D arrays of Ge QDs on patterned Si substrate, exhibiting perfect spatial ordering and size uniformity. QDs prefer to nucleate and grow in convex surface regions where local surface chemical potential is minimum due to maximum strain relaxation. Their idea provides a unique method to guide the self-assembly of QDs by engineering patterned substrates with curved surface of designed convex regions.

III. Publications

The publications supported by the funding are indicated at the end by (DOE).

1. "Equilibrium Shape of Two-dimensional Islands Under Stress", Adam H. Li, Feng Liu, and M.G. Lagally, to *Phys. Rev. Lett.* **85**, 1922 (2000).
2. "Reconstruction of Si(001), (111), and (110) Surfaces", V. Zielasek, Feng Liu, and M.G. Lagally, in "Properties of Crystalline Silicon", the *EMIS* (Electronic Material Information Service) Datareviews, ed. R. Hull, Ch.5.1 (2000) (invited chapter).
3. "Vicinal Si(001) and Si(111) Surfaces", V. Zielasek, F. Liu, and M.G. Lagally, in "Properties of Crystalline Silicon," *EMIS* (Electronic Material Information Service) Datareviews, ed. R. Hull, Ch.5.2 (2000) (invited chapter).
4. "Strain, Morphology, and Self-organization in the Growth of Si/Ge Quantum Dot Nanoclusters", Arthur R. Woll, J. Sullivan, Feng Liu, and Max G. Lagally, in "*Cluster and Nanostructure Interfaces*", ed. P. Jena, S.N. Khanna, and B.K. Rao, 631-638 (World Scientific, 2000). (invited paper).
5. "Evidence for Thermal Roughening of Finite Germanium Layers on Si(001)", J.B. Maxson, D.E. Savage, R. Tromp, M. Reuter, Feng Liu, and M.G. Lagally, *Phys. Rev. Lett.* **85**, 2152 (2000). (DOE)
6. "Magnetization on Rough Ferromagnetic Surfaces", D. Zhao, Feng Liu, D.L. Huber, and M.G. Lagally, *Phys. Rev. B* **62**, 11316 (2000).
7. "Creation of "Quantum Platelets" via Strain-Controlled Self-Organization at Steps", Adam H. Li, Feng Liu, D.Y. Petrovykh, J.-L. Lin, J. Viernow, F.J. Himpsel, and M.G. Lagally, *Phys. Rev. Lett.* **85**, 5380 (2000). (DOE)
8. "Unique Rock-n-Roll Dynamic Appearance of a Si-Ge Ad-Dimer on Si(001)", Z.Y. Lu, Feng Liu, C.Z. Wang, X.R. Qin, B.S. Swartzentruber, M.G. Lagally, K.M. Ho, *Phys. Rev. Lett.* **85**, 5603 (2000). (DOE)

9. "Self-Organized Formation of Nanostructures in Strained Thin Films", Feng Liu, Proceeding of 8th International Conference on Composite Engineering, ed. D. Hui, P. 581 (2001). (DOE) (invited paper).
10. "Pattern Formation via A Two-Step Surface Faceting Transition on Vicinal Si(111) Surfaces", F.-K Men and Feng Liu, *MRS Proceeding*. Vol. 648, P1.7.1-6, (2001). (DOE)
11. "Self-assembly of two-dimensional islands via strain-mediated coarsening" Feng Liu, Adam H. Li, and M.G. Lagally, *Phys. Rev. Lett.* **87**, 126103 (2001). (DOE)
12. "Surface Stress-Induced Island Shape Transition in Si(001) Homoepitaxy" V. Zielasek, Feng Liu, Yuegang Zhao, J.B. Maxson, M.G. Lagally, *Phys. Rev. B (rapid communication)*, **64**, R201320 (2001). (DOE)
13. "Simple Generic Method for Predicting the Effect of Strain on Surface Diffusion", D.J. Shu, Feng Liu, and X.G. Gong, *Phys. Rev. B*, **64**, 245410 (2001). (DOE)
14. "Step-Induced Magnetic Hysteresis Anisotropy in Ferromagnetic Thin Films", D. Zhao, Feng Liu, D.L. Huber, and M.G. Lagally, *J. Appl. Phys.* **91**, 3150 (2002).
15. "Self-Organized Nanoscale Pattern Formation on Vicinal Si(111) Surfaces via a Two-Stage Faceting Transition", F.-K Men, Feng Liu, P.J. Wang, C.H. Chen, D.L. Cheng, J.L. Lin, and F.J. Himpsel, *Phys. Rev. Lett* **88**, 096105 (2002). (DOE)
16. "Nanomechanics: Response of a Strained Semiconductor Structure", Feng Liu, P. Rugheimer, E. Mateeva, D. E. Savage, and M. G. Lagally, *Nature* **416**, 498 (2002). (DOE)
17. "Nanostressors and the Nanomechanical Response of a Thin Silicon Film on Insulator", Feng Liu, M. Huang, P. Rugheimer, D. E. Savage, and M. G. Lagally, *Phys. Rev. Lett.* **89**, 136101 (2002). Featured in Nature Materials Research Highlights (October, 2002). (DOE)
18. Self-Assembly of Three Dimensional Metal Islands: strained vs. nonstrained islands", Feng Liu, *Phys. Rev. Lett* **89**, 246105 (2002). (DOE)
19. "Metal-to-semiconductor Transition in Squashed Armchair Carbon Nanotubes", J.Q. Lu, J. Wu, W. Duan, Feng Liu, B.F. Zhu, and B.L. Gu, *Phys. Rev. Lett* **90**, 156601 (2003). (DOE)
20. "Seeing the Atomic Orbital: first-principles study of effect of tip termination on atomic force microscopy", M. Huang, M. Cuma, and Feng Liu, *Phys. Rev. Lett* **90**, 256101 (2003). (DOE)
21. "The Effect of Island-island Interaction on Coarsening of Strained Islands", Feng Liu, *Jpn. J. Appl. Phys.*, **42**, No. 7B (2003). (Invited Paper) (DOE)
22. "Local-Strain-Mediated-Chemical-Potential Control of Quantum Dot Self-Organization in Heteroepitaxy", Bin Yang, Feng Liu, Arthur R. Woll, Max G. Lagally, *Phys. Rev. Lett* (in press). (DOE)
23. "A Novel Analytical Scheme to Compute the n-fold Convolution of Exponential-Sum Distribution Functions", N.Y. Ma and Feng Liu, *Appl. Math Comput.* (in press). (DOE)
24. "A Geometry Constant Defining Shape Transition of Carbon Nanotubes under Pressure", Ji Zang, Andrejs Treibergs, and Feng Liu *Phys. Rev. Lett* (in press). (DOE)
25. "Computational Study of Metal Adsorption on TiO₂(110) Surface", R. S. Pala, T. N. Truong, and Feng Liu, *Proceedings of ISCANA*. (in press).

26. "Equilibrium Shape of Metal Clusters on Surface", Feng Liu, *Proceedings of ISCANA*. (in press). (invited paper). (DOE)
27. "Mesoscopic modeling and simulation of nanostructure formation on surface", Feng Liu, *Handbook of Theoretical & Computational Nanotechnology*, American Scientific Publishers, (in press) (invited chapters). (DOE)
28. "The Physical Origin of Alignment and Ordering of Si Islands in SOI Agglomeration", Bin Yang, B. Zhang, M. Lagally, G.H. Lu, M.H. Huang, and Feng Liu, *Phys. Rev. Lett* (submitted). (DOE)
29. "Enhancing Surface Reactivity of Transition Metal Oxides by Metal Doping", R. Pala and Feng Liu, *Phys. Rev. Lett* (submitted).
30. "Bending of Films on Ultrathin Substrates", M.H. Huang, Feng Liu, P. Rugheimer, and M.G. Lagally, *Phys. Rev. Lett* (submitted). (DOE)
31. "Self-Organized Growth of Quantum Wire Superlattice in Strain-Compensated Multilayer Film", L. Bai, J. Tersoff, and Feng Liu, *Phys. Rev. Lett* (submitted). (DOE)
32. "Predicting the Adsorptive and Catalytic Properties of Strained Metal Surfaces", R. Pala and Feng Liu, *J. Chem. Phys.* (submitted). (DOE)
33. "Computational Designing of Carbon Nanotube Electromechanical Pressure Sensors", J. Wu, Ji Zang, B. Larade, H. Guo, X.G. Gong, and Feng Liu, *Phys. Rev. B* (submitted). (DOE)
34. "Pressure Induced Hard-Soft Transition of Carbon Nanotubes", D.Y. Sun, D.J. Shu, Feng Liu, and X.G. Gong, *Phys. Rev. B* (submitted). (DOE)

IV. Recognitions/Honors/Awards

- 2001 --- Outstanding Overseas Scholar Award, Chinese Academy of Science
 2002 --- Winner of DOE-BES "Chunky Bullet" competition in Materials and Engineering Physics
 2003 --- Member of the DOE reviewer panel for the Materials and Engineering Physics Research Program at the Sandia National Laboratory, NM.

V. Professional Activities

Invited National/International Conference/Workshop Speaker:

48th Midwest Solid State and Solid State Theory Joint Conference, Grand Fork, ND, Oct. 14-16, 2000

International Conference on Nanostructured Materials, Hong Kong, China, September 8-12, 2000

International Workshop on Materials Modeling and Simulation, Beijing, China, Aug. 21-24, 2000

International Workshop on Surface Growth and Surface Morphology, Israel, June 3-8, 2001 (meeting canceled due to safety consideration)

International Workshop on Nanostructures and Quantum Phenomena, Beijing, China,
June 24-26, 2001

8th International Conference on Composite Engineering (ICCE/8), Tenerife Island, Spain,
August 5-11, 2001

XXXI Winter Meeting on Statistical Physics, Taxco, Mexico, January 8-11 2002

Science Festival for Celebrating 100's Anniversary of Nanjin University, China, May 22-
24, 2002

The 2nd International Workshop on Nanostructures and Quantum Phenomena, Beijing,
China, June 5-8, 2002

The 8th IUMRS International Conference on Electronic Materials (IUMRS-ICEM2002),
Xi'an, China, June 10-14, 2002

The International Workshop on Computational Materials Science, Beijing, China, July 8-
10, 2002

Asia-Pacific Surface & Interface Analysis Conference, Tokyo, Japan, October 1-4, 2002

Workshop on Thin Films and Mechanics (Thin Air Philosophical Socety Symposium),
Laramie, Wyoming, August 4-7, 2003

5th Euromech Solid Mechanics Conference (ESMC-5), Thessaloniki, Greece, August 17-
22, 2003

International Symposium on Clusters and Nano-Assemblies: Physical and Biological
Systems, Richmond, VA, November 10-13, 2003

Invited Departmental Seminar and Colloquium Speaker:

University of Wisconsin-Madison, Materials Science Seminar, March 16, 2000.

University of Wisconsin-Madison, Engineering Physics Seminar, April 10, 2000.

Carnegie Mellon University, Condensed Matter Physics Seminar, May 20, 2000.

University of Utah, Materials Science Seminar, November 16, 2000.

University of Utah, Solid State Seminar, November 23, 2000.

University of Arkansas, Condensed Matter Physics Seminar, April 16, 2001

Harvard University, Materials Science Seminar, April 26, 2001

University of Science and Technology of China, Physics and Chemistry Seminar, June 28, 2001

Institute of Engineering Physics of China, Materials Division Seminar, Chengdu, June 30, 2001

University of Utah, Metallurgical Engineering Seminar, August 28, 2002

University of Wyoming, Mechanics and Materials Seminar, September 13, 2002

Arizona State University, Physics Department Surface Science Colloquium, Tempe, AZ, February 10, 2003

Utah State University, Physics Department Colloquium, Logan, Utah, February 25, 2003

University of Utah, Department of Chemistry, Physical Chemistry Seminar, September 8, 2003

Institute of Theoretical Physics, Chinese Academy of Science, Computational Physics Seminar, Beijing, China, October 9, 2003

University of Wisconsin-Madison, RG Herb Materials Physics Seminar, October 27, 2003

Conferences/Workshops Organizer

APS March Meeting (DCMP Focused Session), Minneapolis, 3/20-25, 2000

International Workshop on Materials Modeling and Simulation, Beijing, 8/21-24, 2000

VI. Degrees earned by students under PI's supervision:

Adam Li, Ph.D., 2000

Yuegang Zhao, M.S. 2001

Minghuang Huang, M.S. 2003

VII. Personnel Supported:

Lugang Bai (graduate student)

Martin Cuma (Research Scientist)

Yong Han (graduate student)

Minghuang Huang (graduate student)

Soenhee Jang (graduate student)

Guanghong Lu (postdoctoral Fellow)