Final Report on
DoE Award DE-FG02-04ER46167 to
Rensselaer Polytechnic Institute

Project title: Control of New Kinetic Barriers & Design of Nanorods
PI: Hanchen Huang

End Date: March 31, 2009

Brief description of accomplishments:

Overall, the accomplishments include three elements.

The first element directly relates to the focus of this project. Specifically, we have determined the three-dimensional Ehrlich-Schwoebel barriers, with and without surfactants [1, 2, and two manuscripts in preparation]; references refer to the list of journal publications. Further, we have discovered a characteristic length scale – the dimension of atomic islands bounded by multiple-layer surface steps [3]. This discovery has made it possible to understand scientifically why nanorods synthesis is possible at all, will enable science-based design of nanorods, and may impact energy technology through nanomaterials design and synthesis.

The second element relates to an exploration – synthesis of nanowires. This exploration is made possible through additional support of a Small Grant Exploratory Research from NSF. Through a combination of atomistic simulations, theories, and experiments, the PI and colleagues have made two contributions to the field. Specifically, they have revealed the physical reason why periodic twins develop during growth of SiC nanowires [4, 5, 6]. Further, they have discovered that SiC nanowire films have an order-of-magnitude higher friction that their macroscopic counterpart [7], something that has never been reported before.

The third elements relates to knowledge dissemination. The PI has co-edited (with Helena van Swygenhoven of PSI) an issue of MRS Bulletin, with the theme of Atomistic Simulations of Mechanics of Nanostructures [8], co-authored a review article

in JOM [9], and authored a review paper in connection with a Banff workshop series co-sponsored by Canada, US, and Mexico [10].

List of journal publications:

1. S. K. Xiang and Hanchen Huang, "Ab initio Determination of Three-dimensional Ehrlich-Schwoebel Barriers on Cu{111}", **Applied Physics Letters** *92*, 101923 (2008).
2. C. G. Johansen, Hanchen Huang, and T. M. Lu, "Diffusion and Formation Energies of Magnesium Surfaces", **Computational Materials Science** (2008) submitted.
3. L. G. Zhou and Hanchen Huang, "A Characteristic Length Scale of Nanorods Diameter during Growth", **Physical Review Letters** *101*, 266102-1-4 (2008).
4. H. W. Shim, Jaron D. Kuppers, and Hanchen Huang, "Strong Friction of Silicon Carbide Nanowire Films", **Nanotechnology** *20*, 25704-1-4 (2009).
5. H. W. Shim, Y. F. Zhang, and Hanchen Huang, "Twin Formation During SiC Nanowire Synthesis", **Journal of Applied Physics** *104*, 63511 (2008).
6. H. W. Shim, J. G. Kuppers, and Hanchen Huang, "High-temperature Stability of Silicon Carbide Nanowires", **Journal of Nanoscience and Nanotechnology** *8*, 3999-4002 (2008).
7. Hanchen Huang and Helena van Swygenhoven, "Atomistic Simulations of Mechanics of Nanostructures", **MRS Bulletin** *34*, 160-163 (2009).
8. F. Sansoz, Hanchen Huang, and D. H. Warner, "An Atomistic Perspective on Twinning Phenomena in Nano-enhanced FCC Metals", an invited paper, **JOM** *60*, 79-84 (2008).
9. Hanchen Huang, "Predictive Modelling of Nanorods Synthesis", **Journal of Physics: Conference Series** *107*, 12006 (2008).

List of participants:

- Hanchen Huang (PI): one month summer salary
- Longguang Zhou (research associate): 80% (the other 20% on development of Monte Carlo method, sponsored by NSF)

- Shikai Xiang (post-doc): full time for half a year (left the PI's group in Oct 2008)
- Hyun Woo Shim (PhD student graduated in 2008): summer support ($8600) only (primarily supported by NSF)
- Christopher Johansen (MS student): materials supply of the value $1500 (he is fully supported by Department of Education GAANN fellowship)