ANNUAL COORDINATION MEETING OF THE DOE COMPUTATIONAL MATERIALS SCIENCE NETWORK (CMSN) on "MULTISCALE STUDIES OF THE FORMATION AND STABILITY OF SURFACE-BASED NANOSTRUCTURES"

October 6-7, 2006

University of Maryland, College Park, MD

Program

Friday, October 6 Morning: CSIC (Computer Science Instruction Center), Room 4122 [CSCAMM Seminar Room]

Session 1 Quantum Growth and Novel Properties of Metallic Nanostructures
Chair: K. M. Ho

8:55–9:05 am	Ted Einstein: Welcome Remarks
9:05–9:15 am	Kai-Ming Ho: Introduction on CMSN and Meeting Technicalities
9:15–9:45 am	Hanno Weitering: Hard Superconductivity in Soft Quantum Films
9:45–10:05 am	Jim Evans: Metal Film Growth on Complex Substrates: 5–fold Surfaces of Icosohedral Quasicrystals
10:05–10:35 am	Jian Shen: Growth and Collective Magnetic Behavior of Interacting Nanodot Assemblies
10:35–10:45 am	*Discussion*
10:45–11:00 am	**Coffee Break**

Session 2 Novel Semiconductor Nanostructures
Chair: E. Kaxiras

11:00–11:30 am	Max Lagally: Latest Fun with Si Nanomembranes
11:30–11:50 am	Kai-Ming Ho: Passivated Semiconductor Nanowires: Structure and Growth
11:50–12:10 pm	Mei-Ying Chou: Electronic and Vibrational Properties of Si Nanowires
12:10–12:30 pm	Feng Liu: Criticality of Morphological Instability of Strained Film Grown on Curved Substrate
12:30–1:30 pm	**Lunch Break (Room 1204 [Toll Room], Physics Building)**

Friday, October 6 Afternoon: Physics Building, Room 1201

Session 3 Molecules on Surfaces
Chair: M. Y. Chou

1:30–1:35pm	Gary Rubloff (Director): Overview of Maryland NanoCenter
1:35–2:05 pm	Zhigang Suo: Competitive Rate Processes and Energetic Forces on Crystal Surfaces
2:05–2:25 pm	Peter Feibelman: Salt Solvation in Ice: Perils of ill-considered MD

2:25–2:50 pm	Tim Kaxiras/Yina Mo: Modeling Growth of Molecular Solids on Inert Substrates
2:50–3:15 pm	Zhenyu Zhang: Hydrogen Science at Nanostructure Surfaces
3:15–3:25 pm	*Discussion*
3:25–3:40 pm	**Coffee Break**

Session 4 Tailoring of Metallic/magnetic Nanostructures
Chair: E. D. Williams

3:40–4:10 pm	Jason Crain: Measuring Electronic Size Effects in Atomic Chains
4:10–4: 40 pm	Michael Aziz: Morphology Evolution Under Ion Sputter Erosion
4:40–5:05 pm	Dio Margetis: Continuum Model of Nanostructure Evolution
5:05–5:15 pm	*Discussion*
5:15–5:45 pm	Jonah Erlebacher: The Dynamic Surface Morphology of Nanoporous Gold
5:45–6:15 pm	Tai Chiang: Surface and Interface Effects in Thin Films and Nanostructures
6:15–6:25 pm	*Discussion*

7:15 pm - Dinner & Reception: Seven Seas Restaurant

Informal after-dinner talk by Bob Park

Saturday, October 7: Physics Building, Room 1201

Session 5 Morphological Evolution and Control
Chair: T. L. Einstein

8:30–9:00 am	Ken Shih: Quantum Size Effects in Metallic Thin Films: From Thermodynamic Stability to Superconductivities
9:00–9:30 am	Michael Tringides: Non-classical Growth Morphologies and Kinetic Barriers in QSE-driven Pb/Si(111) Growth
9:30–9:50 am	Cai-Zhuang Wang: Coarsening and Growth of Quantum Islands
9:50–10:10 am	Ellen Williams: Surface Electromigration: New developments
10:10–10:20 am	*Discussion*
10:20–10:35 am	**Coffee Break**

Session 6 New Approaches of Modeling
Chair: C. Z. Wang

10:35–11:05 am	Talat Rahman: Copper Islands or Catalysis or TBA
11:05–11:35 am	Kristen Fichthorn: Ab initio Kinetic Monte Carlo Simulation of Al(110) Homoepitaxy
11:35–11:55 am	Ram Hariharaputran: Strain-induced Self Organization in Alloy and Multilayer Thin Films – A phase field study
11:55–12:15 pm	Ted Einstein: Scaling of Capture-Zone Distributions: Applying Ideas from Universality of Fluctuation Phenomena to Islanding
12:15–1:30 pm	**Lunch (on own at nearby restaurants)**
1:30–5:00 pm	**CMSN Team: Discussions and Planning**
5:00 pm	**Meeting Adjournment**