

Symposium on Physics and Chemistry of Metallic Quantum Sized Films and Related Nanostructures

November 6 - 8, 2006

Organized by

Department of Physics and The Institute of Theoretical Physics,
The Chinese University of Hong Kong

INVITED SPEAKERS

Tai-Chang Chiang (Univ. of Illinois, Urbana Champion, USA)

Mei-Yin Chou (Georgia Institute of Technology, USA)

Hanno H. Weitering (The University of Tennessee, USA)

Qi-Kun Xue (Tsinghua University, China)

Zhen-Yu Zhang (Oakridge National Laboratory, USA)

Zhong-Xian Zhao (Institute of Physics, CAS, China)

Objective:

To survey and address recent major scientific discovery of quantum growth behavior and the physical properties of simple metal films as a function of the number of atomic layers in the films, so to identify issues on new quantum size effects of selected ultra thin metal films and related nanostructures for future investigation. To provide local faculty members and students an opportunity to gain a deep understanding of the underlying physical mechanisms that governs the relation between quantum electron confinement and properties. To give researchers in the field a platform for exchanging information and ideas that may lead to the development of novel artificial functional materials and devices in many areas of science and technology.

Presentation: Invited lectures

Language: English and Mandarin

Venue: Room 128, Science Centre North Block, The Chinese University of Hong Kong, Shatin, N.T.

Registration: Free; Deadline, October 22, 2006.

Please send email to pyho@phy.cuhk.edu.hk to register. In the email please specify your name, institution, position and contact phone number.

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Program

Time \ Date	November 6 (Mon)	November 7 (Tue)	November 8 (Wed)
09:15 – 09:30	<i>Opening</i>		
09:30 – 10:15	M.-Y. Chou	X. D. Xiao	Round Table Discussion (Chaired by Z. X. Zhao)
10:15 – 10:30	<i>Coffee Break</i>		
10:30 – 11:15	T.-C. Chiang	M.-Y. Chou	
11:15 – 11:30	<i>Coffee Break</i>		
11:30 – 12:15	H. Weitering	Q. K. Xue	
12:15 – 14:00	<i>Lunch</i>		
14:00 – 14:45	T.-C. Chiang	Z. Y. Zhang	
14:45 – 15:00	<i>Coffee Break</i>		
15:00 – 15:45	Z. Y. Zhang	H. Weitering	
15:45 – 16:00	<i>Coffee Break</i>		
16:00 – 16:45	M. Altman	Q. K. Xue	
16:45 – 17:30		J. F. Wang	

Venue: Room 128, Science Centre North Block, CUHK

November 6 (Monday)

- 09:15 - 09:30 *Opening*
- 09:30 - 10:15 **M.-Y. Chou:** Quantum size effects in metal thin films
- 10:15 - 10:30 *Coffee Break*
- 10:30 - 11:15 **T.-C. Chiang:** Quantum size effects in thin films and surface nanostructures
- 11:15 - 11:30 *Coffee Break*
- 11:30 - 12:15 **H. Weitering:** Hard superconductivity in soft quantum films
- 12:15 - 14:00 *Lunch*
- 14:00 - 14:45 **T.-C. Chiang:** Quasiparticles in thin film quantum wells
- 14:45 - 15:00 *Coffee Break*
- 15:00 - 15:45 **Z. Y. Zhang:** Inverse design of surface-based magnetic nanostructures
- 15:45 - 16:00 *Coffee Break*
- 16:00 - 16:45 **M. Altman:** Exploiting quantum well resonances in low energy electron
Microscopy

November 7 (Tuesday)

- 09:30 - 10:15 **X. D. Xiao:** Superconductivity and pseudogap in nanostructured Pb islands
- 10:15 - 10:30 *Coffee Break*
- 10:30 - 11:15 **M.-Y. Chou:** Quantum theory of semiconductor nanowires: First-principles studies of their electronic, vibrational, and optical properties
- 11:15 - 11:30 *Coffee Break*
- 11:30 - 12:15 **Q. K. Xue:** Quantum size effects induced novel properties in Pb thin films
- 12:15 - 14:00 *Lunch*
- 14:00 - 14:45 **Z. Y. Zhang:** Hydrogen science at nanostructure surfaces
- 14:45 - 15:00 *Coffee Break*
- 15:00 - 15:45 **H. Weitering:** Optimal doping control of magnetic semiconductors
- 15:45 - 16:00 *Coffee Break*
- 16:00 - 16:45 **Q. K. Xue:** Spontaneous fabrication of nanocluster arrays on Si(111)
Surface
- 16:45 - 17:30 **J. F. Wang:** Metallic nanostructures

November 8 (Wednesday)

- 09:30 - 12:15 Round Table Discussion (Chaired by Z. X. Zhao)

Abstracts

Monday 9:30 - 10:15 a.m.

Quantum Size Effects in Metal Thin Films

Mei-Yin Chou

School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332-0430, U.S.A.

An intriguing and unexpected feature has recently been discovered during epitaxial growth of metal thin films on semiconductors. Instead of forming three-dimensional (3D) islands of various size as commonly observed for nonreactive interfaces, the metal atoms can arrange themselves into plateaus or islands of selective heights with flat tops and steep edges under certain growth conditions. This extra stability of metal films with specific thickness has an electronic origin, and can be explained by the so-called quantum size effects due to electron confinement. The quantum-well states give rise to an oscillatory behavior in many physical properties as the thickness varies, including the surface energy which determines the stability of the film, the work function which affects the surface adsorption processes, and the superconducting transition temperature. In this talk, I will present our recent density-functional calculations to study these effects in Ag/Fe(100), Pb/Si(111), and various freestanding films. The role played by the substrate and the crystal band structure will also be discussed.

Monday 10:30 - 11:15 a.m.

Quantum Size Effects in Thin Films and Surface Nanostructures

T.-C. Chiang

Department of Physics, University of Illinois, Urbana, IL 61801, U.S.A.

Atomically uniform films of Ag and Pb have been successfully grown on several substrates (Fe, Si, and Ge). The potential barrier at the interface confines the electrons in a film to form quantum well states. The resulting electronic structure of the film can be substantially different from the bulk counterpart, causing the physical properties of the film to vary as a function of film thickness. These variations generally follow a damped oscillatory behavior, and the underlying physics is similar to the shell effect associated with the periodic property variations of the elements in the period table. This talk discusses the basic electronic structure of thin metal films as measured by angle-resolved photoemission and the connections to physical properties including the surface energy, thermal stability, work function, electron-phonon coupling, etc. Interfacial engineering is shown to be an effective means for tailoring the film electronic structure and properties. Quantum size effects can also affect morphological evolution during film growth and heat treatment. X-ray diffraction studies show that the observed development of nanoscale features can be related to the energetics and kinetics of the system.

Monday 11:30 - 12:15 p.m.

Hard Superconductivity in Soft Quantum Films

Hanno H. Weitering

Department of Physics and Astronomy, The University of Tennessee, Knoxville, TN 37996, U.S.A.

Superconductivity is inevitably suppressed in reduced dimensionality. Questions of how thin superconducting wires or films can be before they lose their superconducting properties have important technological ramifications and go to the heart of understanding coherence and robustness of the superconducting state in quantum-confined geometries. In this talk, I will show how quantum confinement of itinerant electrons in a soft metal, Pb, can be exploited to stabilize superconductors with lateral dimensions of the order of a few millimeters and vertical dimensions of only a few atomic layers. These extremely thin superconductors show no indication of defect- or fluctuation-driven suppression of superconductivity and sustain enormous supercurrents of up to 10% of the theoretical depairing current density. Their magnetic hardness implies a superconducting critical state with strong vortex pinning that is attributed to quantum trapping of vortices. Our study paints a conceptually appealing, elegant picture of a model nanoscale superconductor with calculable critical state properties and surprisingly strong phase coherence. Finally, I will show how the quantum growth and superconductive properties of the films can be tailored by Fermi surface engineering, and I will discuss the possibility of multi-gap superconductivity in quantum-confined thin films. This work was done in collaboration with M.M. Ozer, J.R. Thompson, Yu Jia, and Z.Y. Zhang.

Monday 2:00 - 2:45 p.m.

Quasiparticles in Thin Film Quantum Wells

T.-C. Chiang

Department of Physics, University of Illinois, Urbana, IL 61801, U.S.A.

Electrons in thin films can be confined to yield quantum well states. An elementary picture for describing such systems involves a particle confined in a quantum box forming standing waves. The resulting energy levels are determined by the band structure of the film material, which governs the phase of particle propagation. While this model has been very successful in explaining many effects and phenomena, its shortcomings and failures become apparent when one examines in detail the quasiparticle excitation spectra in real thin films as probed by angle-resolved photoemission. Specifically, hybridization coupling of the film states to the substrate states can yield substantial renormalization of the spectral weight function. Most metals films on semiconductor substrates form incommensurate interfaces, and diffraction by the interface potential can be important. These interactions can lead to complex line shapes. Even substrate doping can substantially affect the quantized energy levels. This talk will review some recent results involving Ag and Pb film deposited on Si and Ge substrates.

Monday 3:00 - 3:45 p.m.

Inverse Design of Surface-Based Magnetic Nanostructures*

Zhenyu Zhang

Oak Ridge National Laboratory and University of Tennessee, U.S.A.

Multiscale modeling is gaining an increasingly important role in guiding the fabrication of artificially structured nanomaterials with atomic-scale precision and desirable physical properties. In this talk, a few recent examples will be presented to illustrate its predictive power in modern materials research. The modeling approaches range from electronic-scale calculations based on first principles to mesoscopic-scale continuum elasticity theory. Specific physical systems considered include: (a) fabrication of ordered magnetic atom wires on non-magnetic metal substrates; (b) quantum growth of atomically flat superconducting metal overlayers on semiconductor substrates; and (c) optimal dopant control in dilute magnetic semiconductors via "Subsurfactant Epitaxy". Emphasis will be made on the substantially improved structure-property relationships achieved through such synergetic efforts between theory and experiment, including in the last example the striking observation of magnetic ordering temperatures well above room temperature.

* Supported by USDOE, USNSF, & CAS.

Monday 4:00 - 4:45 p.m.

Exploiting Quantum Well Resonances in Low Energy Electron Microscopy

M. S. Altman

Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong

The physical properties of thin metallic films exhibit remarkable quantum size effects due to the discrete quantum well (QW) states that are caused by electron confinement. Measurements of the elastically reflected electrons from thin films often reveal intensity peaks at very low energy that are associated with QW resonances above the vacuum level. In direct correspondence with the binding energies of QW states below vacuum, the energies of QW resonances are very sensitive to film thickness. This talk will focus on the interpretation of QW resonances and the subsequent three-dimensional view of thin film nanostructure that is obtained from highly laterally resolved measurements of QW resonances in low energy electron microscopy (LEEM). Information on unoccupied band structure and interface scattering phase shifts has been obtained from a phase accumulation model analysis of QW resonances in several thin film systems. Details of the buried interface and strained layer spacings in coherently strained Ag films on the W(110) surface has also been determined accurately by dynamical theory analysis of the intensity peaks associated with QW resonances. Real-time LEEM imaging of Ag films on an Fe(100) surface also reveals novel 'electronic' growth and thermal decomposition morphologies.

Tuesday 9:30 - 10:15 a.m.

Superconductivity and Pseudogap in Nanostructured Pb Islands

Xudong Xiao

Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

Bulk lead (Pb) is a well known superconductor with a transition temperature at 7.2 K. The Pb films grown on Si(111) surface exhibit oscillatory superconducting transition temperature as the film thickness increases layer after layer. What will happen if the lateral dimension of the films is reduced to nanometer scale, below or comparable with the coherent length of superconductivity? Our recent scanning tunneling spectroscopic experiment reveals that a pseudogap develops for these nanometer-sized flat-topped 2D Pb islands. The pseudogap persists to much higher temperatures than the superconductivity transition temperature and have a clear island size dependence. In this talk, I will discuss the relation of the pseudogap with superconductivity and the implication of our observation with the current theory.

Tuesday 10:30 - 11:15 a.m.

Quantum Theory of Semiconductor Nanowires: First-Principles Studies of Their Electronic, Vibrational, and Optical properties

Mei-Yin Chou

School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332-0430, U.S.A.

Nanowires are one-dimensional nanostructures with electrical carriers confined in the other two (perpendicular) directions. They exhibit interesting physical properties that are noticeably different from those of quantum dots and the bulk. In particular, semiconducting nanowires have potential applications in many fields such as optoelectronics, photovoltaic cells, and especially device miniaturization. In order to understand the quantum confinement effect, we have performed calculations of the electronic, vibrational, and optical properties of silicon nanowires using first-principles approaches. Structure relaxation and lattice vibrations are studied within the framework of the density functional theory. The quasi-particle spectra are evaluated using the many-body perturbation theory, and excitonic effects are also included. In this talk, I will report the size and orientation dependence of the band gap, confinement induced vibrational modes, and optical absorption spectra. Of particular interest is the enhanced electron-hole Coulomb interaction in this confined geometry that results in an unusually large binding energy (1-1.5 eV) for the excitons, which dominate the optical absorption spectrum. The current results predict a general features in the optical absorption spectrum of semiconductor nanowires that may impact future applications of these nanostructures.

Tuesday 11:30 - 12:15 p.m.

Quantum Size Effects Induced Novel Properties in Pb Thin Films

Qi-Kun Xue

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Following the textbook description for quantum particles in a box, electrons confined in a perfectly uniform thin film are quantized into discrete energy levels in the vertical direction, forming standing-wave like eigenstates, in analogy with the Fabry-Pérot modes in an optical interferometer [1, 2]. Electron interference is very sensitive to film thickness and smoothness because of the very short wavelength of electron waves (~nanometer) in the case of a metal, and has been proven to modulate electronic distribution near the Fermi level, and thus significantly affect physical and chemical properties of a thin film material [1, 3]. In this talk, we report on such electron wave interference effect on the physical and chemical properties of two-dimensional (2D) Pb thin films on Si(111) substrates.

Using a low-temperature deposition method [4], we were able to grow crystalline Pb films on Si(111) substrate with atomic-scale uniformity in thickness over a macroscopic area, and investigate thickness-dependent quantum size effect on transport properties of the films in a well-controlled manner. Oscillatory superconducting transition temperature, perpendicular upper critical field, local work function [5], thermal expansion, chemical reactivities and giant magnetoresistance effect [6] were observed. Our work clearly demonstrates the possibility of modifying the physical and chemical properties of thin films by exploiting the quantum size effects.

References

- [1] T. -C. Chiang, *Surf. Sci. Rep.* **39**, 181 (2000).
- [2] J. J. Paggel, T. Miller, T. -C. Chiang, *Science* **283**, 1709 (1999).
- [3] C. M. Wei and M. Y. Chou, *Phys. Rev. B* **66**, 233408 (2002)
- [4] A. R. Smith et al., *Science* **273**, 226 (1996); Z. Zhang, Q. Niu, C. K. Shih, *Phys. Rev. Lett.* **80**, 5381 (1998).
- [5] Y. Guo et al., *Science* **306**, 1915 (2004); X. Bao et al., *Phys. Rev. Lett.* **95**, 247005 (2005); Y. F. Zhang et al., *Phys. Rev. Lett.* **95**, 096802 (2005).
- [6] Xu-Cun Ma et al., (unpublished).

* In collaboration with Jin-Feng Jia, Xucun Ma, Lu Li, X. C. Xie, E. G. Wang, Z. X. Zhao (IOP), Wenhui Duan (Tsinghua), Qian Niu (UT Austin), Z. Q. Qiu (UC Berkeley), and F. Liu (Utah). The work was financially supported by Ministry of Science and Technology and NSF of China.

Tuesday 2:00 - 2:45 p.m.

Hydrogen Science at Nanostructure Surfaces*

Zhenyu Zhang

Oak Ridge National Laboratory and University of Tennessee, U.S.A.

As one of most affluent elements in nature, hydrogen is gaining increasing attention in our search for clean energy. In order to eventually realize the ultimate dream of using hydrogen as a primary fuel cell, how to store and retract hydrogen are critical steps. In this talk, I will present some latest results from preliminary studies of a few elemental processes related to hydrogen storage. The focus is on how hydrogen interact with the surfaces and interfaces of artificially structured nanomaterials. Such understandings should be helpful in our search for optimal hydrogen storage media.

* Supported by USDOE, USNSF, & CAS.

Tuesday 3:00 - 3:45 p.m.

Optimal Doping Control of Magnetic Semiconductors

Hanno H. Weitering

Department of Physics and Astronomy, The University of Tennessee, Knoxville, TN 37996, U.S.A.

In this talk, I will discuss a discovery that is expected to have due impacts in two forefront areas of materials research. First, I will introduce "subsurfactant epitaxy" as a novel kinetic pathway toward the synthesis of non-equilibrium structures and materials. The discovery of subsurfactant growth is of broad fundamental- and paramount practical interest, particularly within the context of doping functional materials. Secondly, we have successfully applied this conceptual advance to alleviate a major bottleneck problem in spintronics, namely how to fabricate dilute magnetic semiconductors with ferromagnetic ordering temperatures that exceed room temperature by a comfortable margin while minimizing the structural disorder and inhomogeneities that are intrinsic to high doping levels. Detailed comparison between Mn-doped Ge samples grown by conventional MBE and samples grown via the subsurfactant procedure indicates the vastly superior structure-property relationship of the latter. Finally, I will present a detailed analysis of the magneto-resistance and anomalous Hall effect as a function of the dopant distribution in these materials. This work was done in collaboration with C. Zeng, A.P. Li, L.C. Feldman, and Z.Y. Zhang.

Tuesday 4:00 - 4:45 p.m.

Spontaneous Fabrication of Nanocluster Arrays on Si(111) Surface

Qikun Xue

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Metal nanodot ordered arrays are promising material for next generation microelectronics, ultra-high-density magnetic recording, and nanocatalysis. Self-organization in heterogeneous strained thin film growth and self-assembly in chemical synthesis are two of the most commonly used methods to obtain such nanostructures. However, none of these methods have succeeded in producing identical nanodots with a periodic spatial distribution.

In this work, ordered arrays of metal nanoclusters were fabricated by using a novel technique, in which metal surface-mediated magic clustering is used to achieve the identical dot size while the Si(111)-7×7 surface as a template for positioning them in order. The atomic structures, formation mechanism and stability of the nanoclusters were studied with *in-situ* scanning tunneling microscopy observation combined with first-principles total energy calculations. The versatility of this method is demonstrated with various metals, such as group III and magnetic (Mn and Co) metals.

References

- [1] J. L. Li et al., *Phys Rev. Lett.* **88**, 066101 (2002)
- [2] J. F. Jia et al. *Appl. Phys. Lett.* **80**, 3186 (2002)
- [3] J. F. Jia et al., *Phys. Rev.* **B66**, 165412 (2002)
- [4] M. H. Pan et al., *Nano Letters* **5**, 87 (2005)

* In collaboration with Jin-Feng Jia (IOP, China), Shengbai Zhang (NREL, USA) and Zhenyu Zhang (ORNL, USA), X. R. Wang (HKUST, China), C. K. Shih and J. T. Markert (UT Austin).

Tuesday 4:45 - 5:30 p.m.

Metallic nanostructures

Jianfang Wang

Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong

Metallic nanostructures have great potentials in optical, electronic, and biotechnological applications due to their rich surface plasmon-related optical properties. The surface plasmon resonance wavelengths of metallic nanostructures can be tailored from the visible to infrared spectral regions. The light within the near-infrared region of 800 - 1300 nm can penetrate biological tissues with relatively high transmittivities. Moreover, metallic nanostructures exhibit local electric field enhancement at their surface plasmon resonance wavelength, which can be used to improve device performance and detection sensitivity through modification of light-matter interactions.