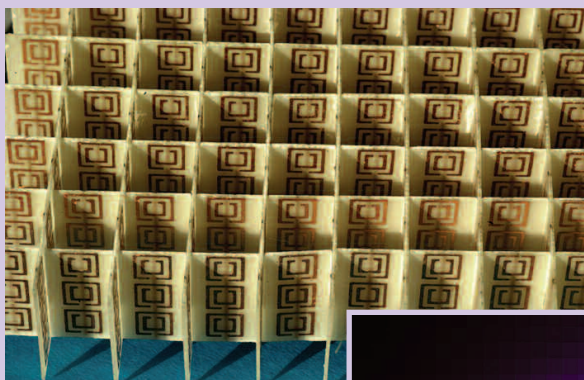
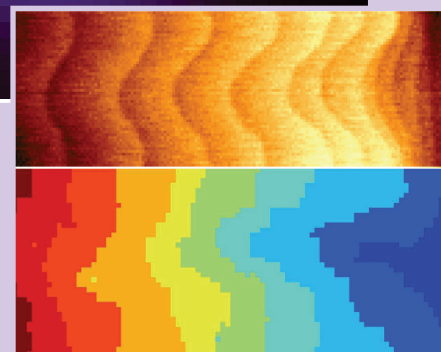


**Imperial College
London**



The Blackett Laboratory

Condensed Matter Theory



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Nanoscale and mesoscale materials physics
Complexity science
Theory and simulation of materials
Quantum Monte Carlo simulations
Quantum phases of matter
Nanophysics and disorder
Metamaterials and negative refraction

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Developments in nanotechnology provide new opportunities for theorists to test our fundamental understanding of condensed matter and to conceive new materials for innovative applications. New physics arises at the nanoscale whenever the size of a sample become smaller than characteristic length scales of particular phenomena and processes. For example, Ohm's law eventually breaks down in a copper wire as the size of the wire becomes less than the distance an electron travels before it loses its energy through scattering by atomic vibrations or other electrons. The correlated nature of the motion of electrons to minimize the repulsion stemming from their charge and spin may become very marked in nanostructures producing new phenomena such as Coulomb blockade. In optics the electromagnetic fields near to an object contain more information about the object than those that have propagated further. This is because at distances large compared to the wavelength of the radiation the near field has decayed leaving only the far-field solutions of traditional optics. But we have conceived a new class of man-made *metamaterials* that has the potential to transmit the near-field as effectively as the far-field, enabling a perfect image of the object to be constituted, at least in principle. This has led to the concept of the perfect lens, free from the usual limit to spatial resolution of the wavelength of the radiation. The trick to the transmission of the near-field is the coupling of surface plasmon resonances excited on nanostructures within the metamaterial.

Self-assembly is widely used to create patterned nanostructures, such as uniform arrays of regularly spaced quantum dots (nanoscale islands of some material) on a substrate. The theory underlying self-assembly and pattern formation involves the statistical mechanics of non-equilibrium systems, and the science of complexity which treats the emergence of patterns at a hierarchy of larger length scales as a result of many interactions at smaller length scales.

Our work on complexity spans all length scales from nanostructures to earthquakes and the engineering of reservoirs. By establishing rigorous links with well-established concepts of equilibrium statistical mechanics, such as universality and the renormalisation group, we are developing new theoretical tools to treat non-equilibrium systems, including certain self-assembled nanostructures.

Science of Complexity

K Christensen

Recently, the science of complexity has enjoyed intense activity across a variety of scientific disciplines. In particular, much progress has been made through the application of tools from statistical physics and critical phenomena in equilibrium systems to study complexity. The overall objective of the science of complexity is to address why non-equilibrium systems often are associated with emergent properties such as simple patterns, hierarchical structures, fractal structures, and other scale-free behaviour.

Science of Complex Networks

K Christensen and N Farid

We are investigating models numerically and analytically addressing possible fundamental mechanisms of the growth and evolution of biological networks. The aim of the research is to ascertain whether dynamical networks can self-organise into a state with large-scale statistical properties, such as scale-free degree distributions as observed in nature.

Universality in Systems Displaying Self-Organised Criticality

K Christensen and M Stapleton

Universality is a very powerful concept in critical phenomena in equilibrium systems and it is believed that similar principles apply to non-equilibrium systems. We have been studying universality in simple non-equilibrium systems displaying self-organised criticality. The emphasis of the work is to gain an understanding of the origin of universality in models where analytical solutions are available.

Upscaling of Reservoir Properties

K Christensen, P King and V Pancaldi

Upscaling is needed when large quantities of data are integrated into a coarse model, preserving heterogeneity and highlighting the large-scale behaviour of the system, for example in reservoir engineering and in any field where all length scales are important. A new simpler and faster method has been devised for upscaling based upon the concept of the renormalisation group transformation from critical phenomena in equilibrium systems.

Quantum Mechanical Modelling of Solids

W M C Foulkes, N D M Hine, J Le Page and A Sorouri

Most of the properties of everyday materials depend on the quantum mechanics of the electrons they contain. The density of a solid, for example, is fixed by a balance between the quantum mechanical kinetic energy of the electrons, which favours low density, and the electrostatic attraction between the nuclei and electrons, which favours high density. Without quantum mechanics, even the simplest properties of the most familiar objects are inexplicable.

Solids can be modelled quite accurately using only a thousand or so electrons, but the resulting 3000-dimensional many-electron Schrödinger equation presents a formidable mathematical challenge. The standard approach is to use mean-field approximations to separate the Schrödinger equation into 1000 single-electron equations. This trick has proved outstandingly successful, but fails qualitatively in strongly correlated materials and quantitatively in many other cases. Our quantum Monte Carlo (QMC) techniques use mean-field theory as a starting point, but go further to include a realistic description of the electron-electron interaction. This year we completed the first accurate QMC calculations of the surface energies of simple model solids, explaining the disagreement between the results of previous QMC simulations and other methods. We

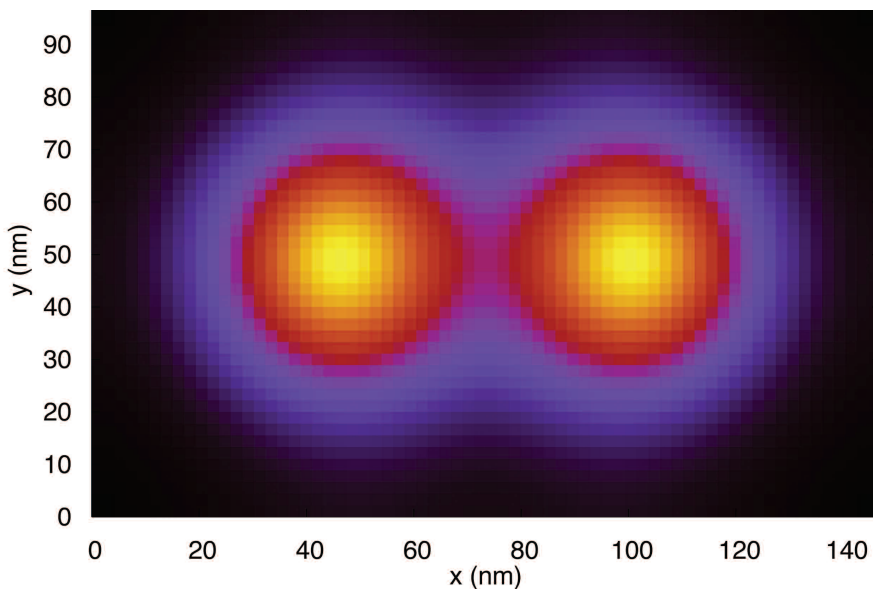


Figure 1. Electron density for the singlet state of a quantum dot molecule with two electrons. The coupled spins of the two electrons have been proposed as a practical realization of qubits for quantum computing.

have also constructed a database of accurate exchange energy densities for a wide variety of realistic model solids, which will be used to improve the exchange-correlation energy functionals used in mean-field calculations. New projects include a QMC study of quantum dots (see Figure 1).

Quantum Phases of Matter

D K K Lee

When we put together a large collection of atoms or electrons, order may emerge from their complex cooperative behaviour. Examples include superconductivity and ferromagnetism. A central challenge in condensed matter physics is the question: *how does the sum become more than its parts?* These emergent phenomena can give rise to new possibilities in the design of new materials and devices.

Superfluidity for Electron-Hole Pairs and in Ultracold Atomic Mixtures

D K K Lee, T Duric, O Garcia Cantú Ros and A Ho

Electrons and holes can become bound pairs, called *excitons*. It has been speculated that they can condense into a superfluid state, but this remains elusive. A recent candidate is the *quantum Hall bilayer*. This system consists of two layers of electrons in close proximity on the nanometre scale, in a strong magnetic field. There have been tantalising experiments pointing to exciton superfluidity: if we inject opposite currents in the two layers, there appears to be little dissipation.

These bilayers also violate Ohm's law for electrical conduction which states that the current should be proportional to the driving voltage. Surprisingly, the current across the bilayer appears to increase when the voltage is decreased! Our group was the first to explain this phenomenon by showing that the loss of quantum coherence in this system is the key to this puzzle.

Our goal is to test theoretical expectations for excitonic superfluids against new experimental results. The underlying physics is also relevant to the study of ultracold atomic mixtures. From a wider perspective, this system provides a testbed for ideas about coherence and decoherence in materials which are candidates for nanotechnological applications.

Nano-Electro-Mechanical Systems (NEMS)

A MacKinnon

When devices are reduced to the scale of a few tens of nanometres there can be profound changes in their behaviour associated with quantum behaviour of the mechanical aspects of the system. While there are many possible such devices we have concentrated our efforts on a simple model electromechanical system: the quantum shuttle (see Figure 2). A quantum dot is situated between 2



Figure 2. The quantum shuttle – a model electromechanical system.

leads and is free to move between the ends of the leads, subject to a spring. When the dot is close to a lead an electron can tunnel freely between the dot and the lead, but when the dot is further away the barrier to tunnelling becomes too large. In such a system the main mode of transport is 'shuttling' in which the dot oscillates between the 2 contacts carrying a single electron across per cycle. The system can be driven as long as the difference in chemical potential between the 2 leads is sufficient to generate a phonon.

Nano-Spintronics

A MacKinnon

There is much current interest in the possibility of manipulating a current of spin polarised electrons, especially in the context of quantum computing. When electrons are confined on the nanoscale an additional relativistic contribution (the Rashba term) to the Hamiltonian makes it possible to separate the current into spin-polarised contributions even in the absence of magnetic materials. At a T-junction, for example, an unpolarised current in the vertical lead gives rise to spin-polarised currents in the cross branches. Related phenomena can be observed in other structures.

Metamaterials for Near-Field Optics

J B Pendry, M C K Wiltshire, B Wood and J Li

The near field is the awkward customer in electromagnetism: it refuses to radiate away from objects and therefore cannot be captured by a conventional optical system. Locked away in the near field are the fine resolution details of the object and their absence from a conventional image limits resolution to about a wavelength. New technology is enabling us to manufacture a class of electromagnetic materials engineered on a scale much less than the wavelength, so that the structure is invisible to radiation. The new materials have properties not seen in nature, such as a negative refractive index, which are the key to controlling the near field (see Figure 3). They imply short wavelength resonances on the surface which couple to and capture the near fields on neighbouring surfaces. Most of the demonstrators have operated in the GHz region of the spectrum where

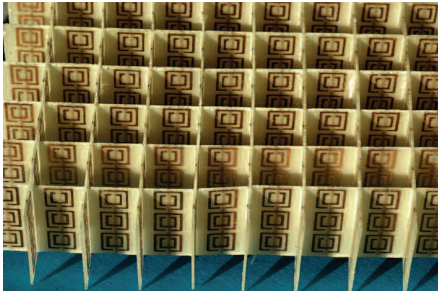


Figure 3. A split ring structure etched into copper circuit board plus copper wires to give negative ϵ and negative μ . The cell side is approximately 10mm and the operating frequency around 10GHz. Structure made at UCSD by David Smith to a design by our group.

the engineering is easier, but structures exhibiting magnetism at THz frequencies have been built and at optical frequencies metamaterial designs exploiting the plasma resonances of a free metal surface are waiting to be exploited.

Theory of Quantum Dot Formation on Singular and Patterned Substrates

D D Vvedensky and C Haselwandter

Self-organization in heteroepitaxial systems has been the subject of numerous theoretical studies, but there is no general methodology that captures the essence of thin film evolution in the presence of lattice misfit in specific materials systems. We have derived a stochastic differential equation for the morphological evolution of heteroepitaxial surfaces from an atomistic model for coherent 3D island formation. Our approach is based on transforming the master equation, which is statistically equivalent to kinetic Monte Carlo simulations, into a formally exact lattice Langevin equation, and then to a stochastic differential equation. The form of our equation is similar to that obtained from continuum elasticity, but the coefficients embody the atomistic ancestry of the processes in the model, which permits a materials parameterization. Comparisons with experiment (from Eli Kapon's group at EPFL) are being carried out to determine the surface morphology for particular scenarios.

Step Morphology on Patterned Substrates

D D Vvedensky

The lithographic patterning of surfaces exposes facets with different chemical, transport, and structural properties. These differences can be exploited to provide control over the spatial positioning of nanostructures and their size uniformity during epitaxial growth. An especially striking consequence of facet interactions is the morphology of steps on (001) mesas on V-grooved GaAs surfaces, as shown in figure 4. A model of steps on such mesas reveals that the conditions for such a profile are (i) reflecting boundaries at the edges of the V-groove, and (ii) preferential diffusion along the step edges of the deposited species. The implications of this model are being explored for the controlled fabrication of nanostructures on these surfaces.

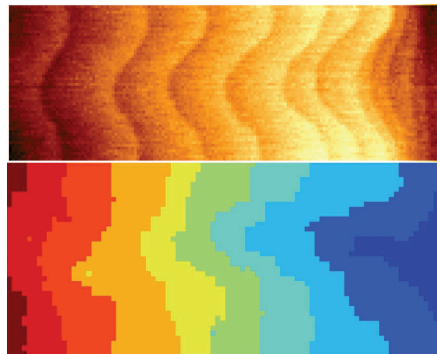


Figure 4. (top) Atomic force microscope image of steps on a V-grooved GaAs surface. (bottom) Simulation of growth on a V-grooved surface.

Nanoscale and Mesoscale Materials Physics

A P Sutton

Our research addresses the fundamental physics underpinning aspects of nanotechnology and other technologies that depend critically on materials

Dynamical Simulations of Non-Adiabatic Processes

A P Sutton, W M C Foulkes, M W Finnis, D R Mason and J Le Page

Irreversible exchanges of energy between electrons and nuclei are being modelled dynamically with a new formalism, 'correlated electron-ion dynamics', in collaboration with colleagues at UCL and Queen's

University Belfast forming a £1.2M consortium funded by EPSRC. We are focussing on non-adiabatic processes that occur when high energy particles impact on metals and create 'radiation damage'. The consortium is also addressing Joule heating in metallic nanowires and electronic transport processes in polymers.

Magnetoelasticity and Magnetoplasticity

A P Sutton, S L Dudarev and M Kurdian

The influence of magnetism on the energies of formation and interaction of defects in ferromagnetic iron is being studied through the development of new interatomic forces that take magnetic spins into account. This work is motivated by the proposed use of ferromagnetic iron in steels to line the walls of a fusion nuclear reactor.

Mesosopic Simulations of Polymers

A P Sutton, D R Mason and S Sabetazad

We are developing a coarse-grained model of polymers for dynamical simulations of processes such as fracture of polymer-inorganic interfaces. The central idea is to model a polymer chain as a flexible inextensible wire, with bending and twisting elastic moduli, that interacts with itself and other polymer chains through Lennard-Jones potentials. A principal objective is to model reptation and disentanglement processes during fracture. Another is to generate realistic polymer conformations for simulations of electronic transport.

Confined Liquids

A P Sutton, M W Finnis, G Pruessner, S von Althan and K Kaski**

When liquids are confined spatially at the nanometre scale they inherit some of the structure of the confining walls. They then cease to behave in the same way as normal liquids, e.g. they may be less effective as a lubricant. Interfaces in ceramic materials may comprise a confined disordered film of nanometre scale thickness, depending on the thermodynamic conditions. The structures of interfaces in Si and perovskite materials are being studied as a function of temperature and oxygen partial pressure as part of an EU-funded consortium involving 6 European centres.

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