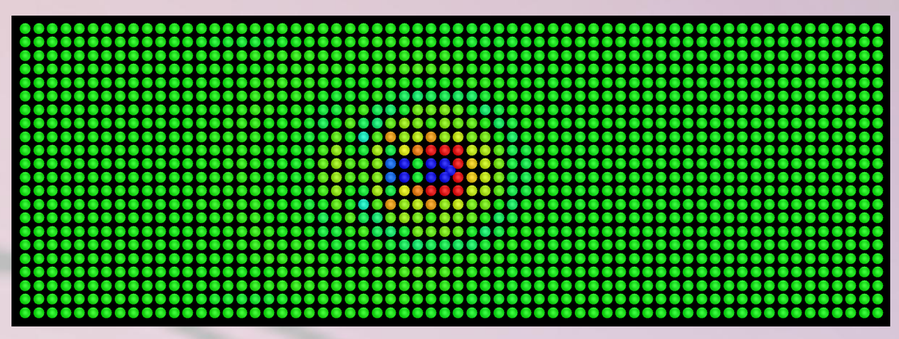
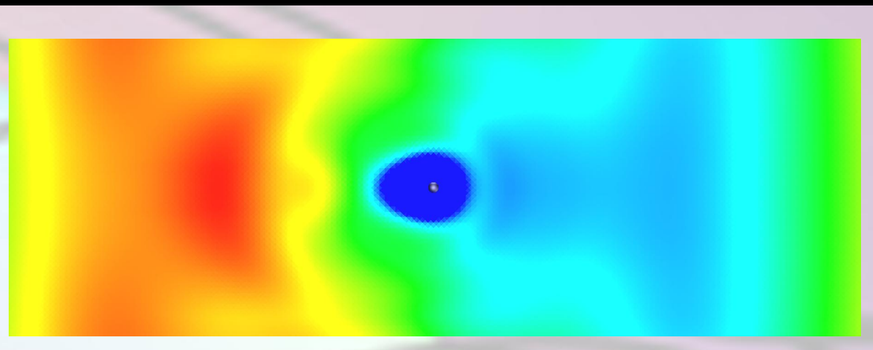
Imperial College London

Doctoral Training Centre

Theory and Simulation of Materials

If you relish the challenge of understanding mathematically complex physical phenomena, and you want to apply your talent for theory to address some of the most significant issues faced by modern society, read on. It is hard to think of a single modern technology that is not completely dependent on materials. The production of energy, telecommunications, aerospace and land transportation; the storage, processing and transmission of information; healthcare; security and defence and more, are all dependent on materials. Our ability to use theory and simulation to guide the selection of materials, to optimise design and performance, and to predict and avoid failures are crucial to all these technologies. Theory and simulation also enable us to think the unthinkable, to create entirely new classes of materials such as materials to render objects invisible. The emphasis in this Doctoral Training Centre (DTC) is on creating new models, new theory and new computational algorithms at the frontiers of materials research, as in the surrounding examples. The PhD projects of the DTC will be carried out in the Thomas Young Centre (TYC) – the London Centre for Theory and Simulation of Materials (TSM).



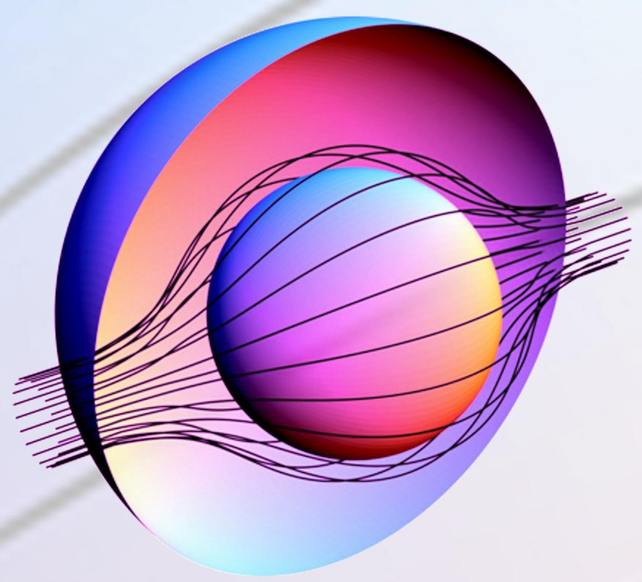


Radiation damage simulation: a 1 MeV ion moves left-to-right down a <100> channel in copper, simulated using time-dependent tight-binding in a simulation cell of 14080+1 ions. Above: the on-site ionic charges show the negatively charged ion is ahead of the compensating screening charge cloud. Below: the Hartree potential in the plane shows a gradient against the direction of motion, indicating a Coulomb drag force.

PURPOSE OF THE TSM DTC

The TSM-DTC has been set up this year to meet the national and international need for mathematically strong physical scientists and engineers with advanced skills in the theory and simulation of materials. The aim of the DTC is to train physical science and engineering postgraduates to carry out cutting-edge multi-disciplinary research in TSM.

The central theme is *bridging length and time scales* since the need to bridge scales poses some of the most challenging problems in TSM. Students will be given a broad foundation in theoretical materials physics together with techniques of simulating materials across the wide range of length and time scales that are likely to be met in industrial and academic research.



Metamaterials: it has recently been noticed that the optical properties of a material may be tailored by adjusting its microstructure as well as its chemistry. Simulation has been used to design such metamaterials, which can even be made to have a negative refractive index. Applications include a perfect lens and an electromagnetic cloak, depicted above.

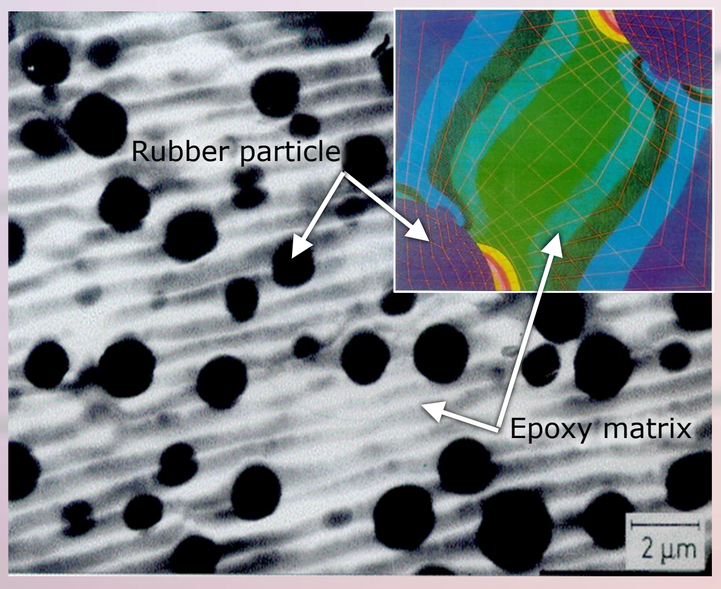
THE DTC EXPERIENCE

This DTC will provide a cutting-edge educational and research environment in TSM across length and time scales, spanning the disciplines of physics, materials, chemistry and mechanical engineering to enable students to learn to view materials problems from different perspectives.

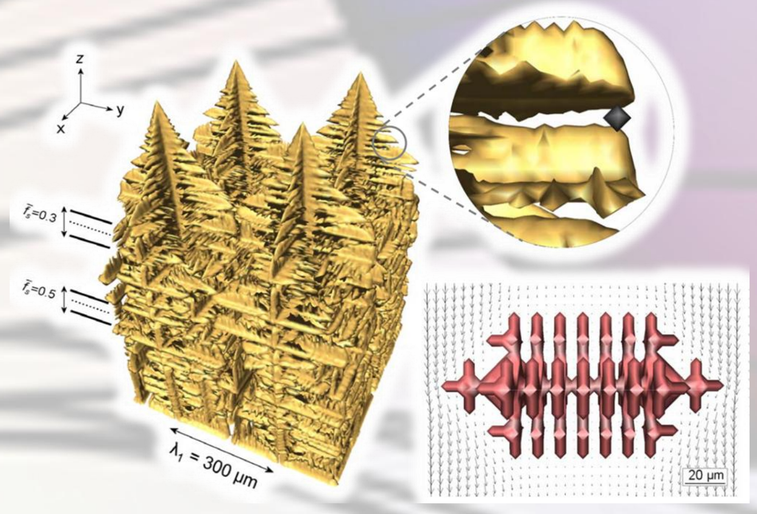
To achieve this, the first year will provide a rigorous training in the required theoretical methods and simulation techniques through the new MSc course in TSM. The PhD research project, which will occupy years 2-4, will have two supervisors (one of whom may be in industry or at another university) whose combined expertise will bridge multiple length and time scales. A key emphasis of research projects will be on the development and implementation of new theory and code for materials simulation.

Other activities that each cohort of DTC students will participate in and benefit from include:

- weekly tea and talk with the Cohort Mentor
- monthly Journal Club
- MSc conference at the end of year 1
- annual Computational Methods workshop
- award-winning transferable skills courses
- seminars, workshops and soirees of the TYC
- annual DTC Open Day and Conference



Rubber toughened epoxy adhesives: when the material is stressed (e.g. at a crack tip), there will be triaxial tensile stresses acting on the rubber particle due to the different elastic moduli and Poisson ratios of the rubber particle and the surrounding matrix. This leads to cavitation of the rubber particles which enables plastic void growth, and hence a large increase in the toughness. Such materials are being used in the Airbus A380 'superjumbo'. Inset: the stress field.



Microstructure prediction: superalloys have very inhomogeneous microstructures containing features such as 'freckles' that cause creep and fatigue failure. Multiscale simulation methods have been applied to model the solidification process, improving predictions of freckle formation.

THE MSc COURSE: YEAR 1

The first year is a 12-month, 90-ECTS, Bologna-compliant MSc in the Theory and Simulation of Materials. This course provides a foundation in theoretical materials physics and its applications in simulations across length and time scales.

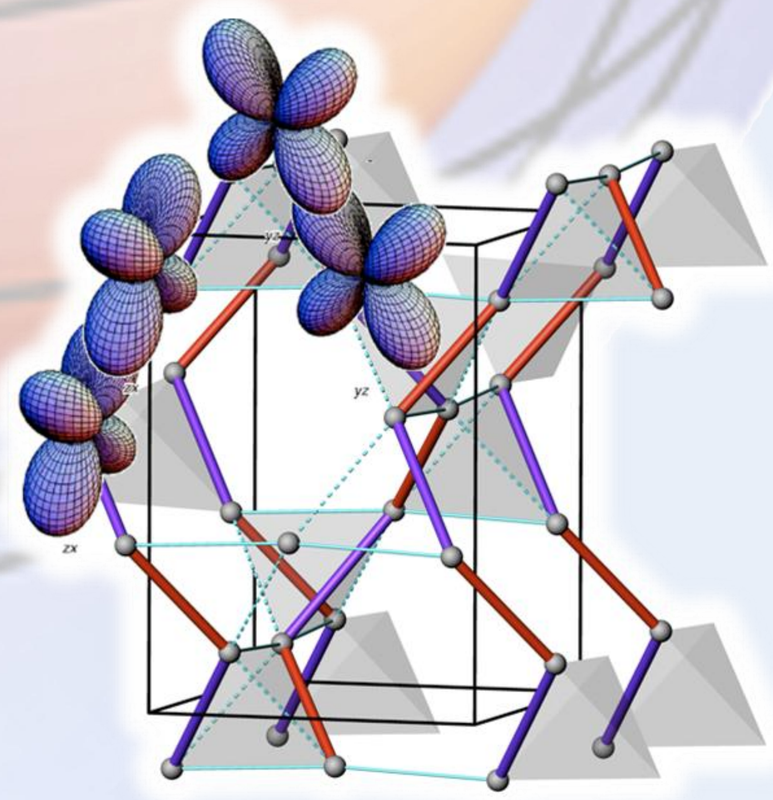
There are six core courses:

- Mathematical and Computational Methods
- Equilibrium in Materials
- Change in Materials
- Electronic Structure of Materials
- Elasticity and Microplasticity
- Materials Simulation from Electrons to Finite Elements

Students will also select two options in the first year and may take further options in later years. Possible options include:

- Methods of Characterising Materials
- Advanced Continuum Theories of Microstructural Evolution
- Polymers and Soft Condensed Matter Physics
- Advanced Continuum Field Theory of Defects
- Strengthening Mechanisms and Fracture
- Advanced Electronic Structure & Metamaterials
- Continuum Theory of Static and Dynamic Plasticity
- Advanced Techniques of Materials Simulation

For both the core courses and options, the teaching involves a mix of lectures, directed reading, problem classes, computational exercises and seminars.



First-principles quantum-mechanical calculations: when doped with magnesium TiO_2 forms the cubic $MgTi_2O_4$ phase. The electrons donated from the Mg ion are predicted to localise strongly in particular Ti-*d* orbitals. The localised electrons interact strongly to form a beautiful orbitally ordered chiral spin phase which has been observed in neutron diffraction experiments. The bonds distort from the cubic structure to form alternating short (purple) and long (red) bonds due to the alternating orbital occupancy.

HOW TO APPLY

Prospective applicants are encouraged to make informal enquiries by contacting the Admissions Tutor Dr. Peter Haynes. Applications must be made through the Department of Physics.

Applicants should have, or expect to achieve, a first class Bachelor's or Master's degree in the physical sciences or engineering. The selection procedure will include an interview with members of the Research Board of the TSM-DTC.

The DTC has funding from the EPSRC for up to ten four-year PhD studentships per year. This funding may be used to pay the fees of students from the UK and EU, and also the stipends of students who have been "ordinarily resident" in the UK for the last three years.

Applications from students with their own funding are welcomed. Imperial also has a number of scholarships for postgraduate study.

EPSRC Engineering and Physical Sciences Research Council