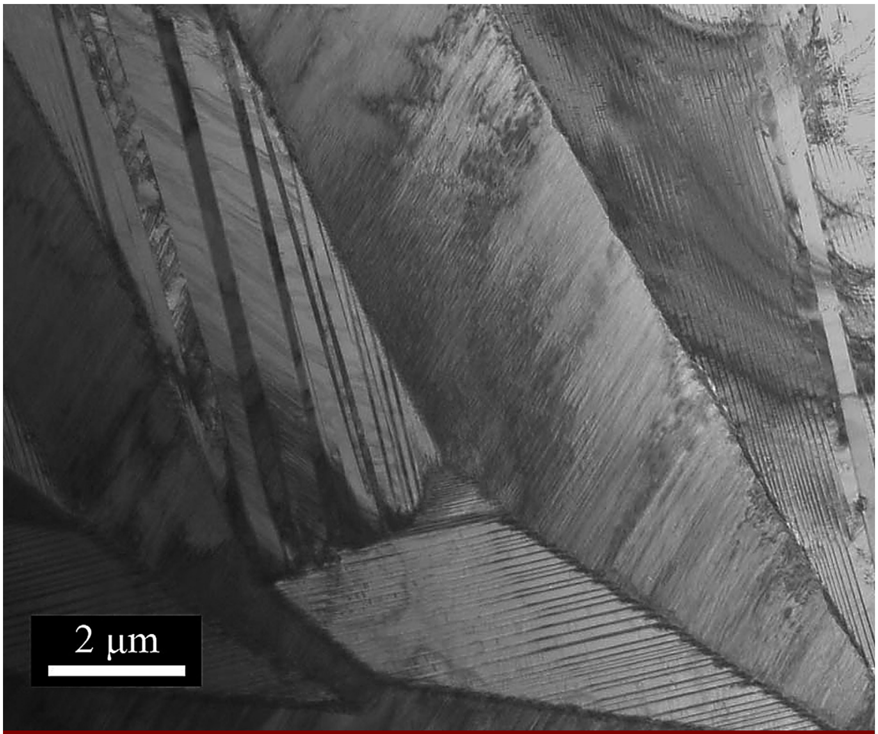
The potential of 'smart' materials is enormous. Deepening our understanding of the related solid-to-solid phase transformations will allow us to extend the range of possible applications still further, says **Nick Schryvers** of the MULTIMAT project

Multi–scale modelling brings multiple benefits



RO2 centres on detailed investigation of the symmetry properties of crystalline materials

Many of the current problems in advanced functional materials are directly related to the wide range of length and time scales involved in the phase transformations that occur in them.

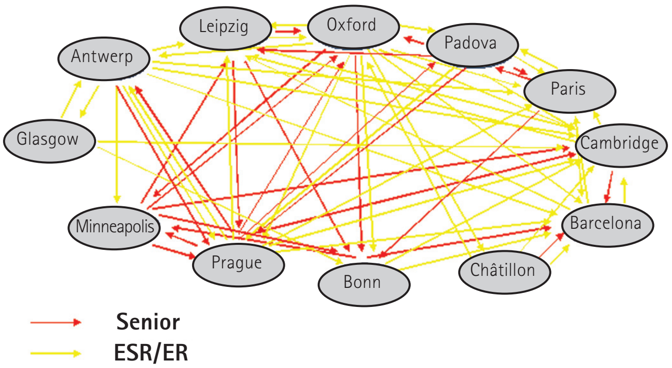
With this issue firmly in mind the MULTIMAT project (Multi-Scale Modelling and Characterisation for Phase Transformations in Advanced Materials), a Marie Curie research and training network comprised of some 12 partners from across Europe, was formed in 2004 with the express goal of building, organising and applying a dedicated constellation of training and mobility opportunities to bring together and educate young European scientists in the multi-scale modelling and characterisation of functional materials like shape memory alloys. The MULTIMAT project includes experts in mathematics, mechanics, physics, and materials science. This makes it one of the broadest networks to receive direct funding from the European Union Framework Programmes.

The scientists and trainees participating in MULTIMAT typically share a number of interests – including the phase transformational aspects of advanced materials, the prediction of their properties, and the development of their potential applications – across the entire nano-, micro- and meso-scale range. Bridging the gap between the different scales that characterise transition phenomena in materials remains a very challenging research problem. Indeed, modern experimental and theoretical investigations require dedicated training and a strong focus beyond the classical educational schemes. Training in the MULTIMAT project is primarily focused on early-stage researchers (ESRs) with less than four years of research experience. In most cases it is strongly related to a doctoral thesis, while transfer of knowledge is closely associated with the experienced researcher's (known as ERs – with either four to 10 years of experience or a PhD) work plan. Both the ER and ESR are explicitly exposed to the wide variety of research methods and results related to their field, even those obtained by other network contractors. This is a particularly important attribute given that MULTIMAT draws much of its strength from the experiences of a previous European network which included many of the same teams. The project has thus achieved a high degree of cohesion and convergence between its various teams in terms of research methods, activities and goals.

By the end of the four years of the MULTIMAT project, 18 ESR and 17 ER positions will have been occupied. Currently, researchers from the Ukraine, Armenia, China, Kenya, Brazil and Mexico undertake around a quarter of the network's workload in terms of time, while researchers from European member states are responsible for the remainder. Experience has told us that this kind of approach represents a good geographical balance. For example, the coordinating team – the University of Antwerp – welcomed one female ER from the Czech Republic, two young male ESRs from Romania and France, and one female Chinese ESR, while gender equal opportunity measures are also applied. However, this last aspect is not always apparent due to the predominance of male researchers in our network's typical disciplines.

The MULTIMAT network is very active in terms of both training and transfer of the researchers' knowledge. This latter goal is furthered by in-house activities, network activities and participation in external events. During their fellowship researchers are encouraged to visit other teams for either short terms or longer secondments, while senior researchers are often invited to visit other teams within the network. Every six months a network meeting takes place at one of the contractor sites at which both researchers and former researchers make a brief presentation of their work. At the same time, Introductory and Intensive Courses are organised and presented by senior team members or external specialists in order to introduce the ESR and ER to both the existing and new techniques available. The members of our different teams have already published over 40 joint papers in peer reviewed journals. This number is increasing every year, while many more conference contributions have also been presented.

As for the actual research, four major research objectives (ROs) have been defined within the network, with several tasks and milestones identified within each RO. By their involvement in several of the ROs and tasks, the research teams generate a lot of new interactions, especially among the young researchers. The themes and contents of the ROs focus on multi-scale modelling and the characterisation of functional materials and their phase transformations. Typical examples of these are martensitic and related transformations, such as those appearing in the shape memory and superelastic systems applied in stents and orthodontic wires. Our primary ROs are outlined below:



Visits by MULTIMAT researchers to other teams involved in the project indicating high frequency and good coverage

RO 1

Improving materials characterisation and understanding. This involves the characterisation of representative materials and model systems by advanced experimental techniques and the interpretation of the obtained data in terms of mathematical and theoretical models.

This RO focuses on the application of highly advanced characterisation techniques to the chosen problems in the phase transformations of interest. The groups involved develop novel experimental techniques like highly advanced transmission electron microscopy (TEM) or X-ray diffractometry methods in-house. This leaves the groups ideally placed to apply them to actual cases, preferably with the emphasis on acquiring quantitative data. Dedicated in-situ characterisation experimentation of phase transformations – under applied stress for example – is another issue under particularly close examination in this RO. The choice of materials ensures direct collaboration with those teams not involved in materials characterisation, while there is also significant input from the mathematical and theoretical models developed and provided by the other teams with regards to the design of the experiments and interpretation of the generated data.

RO 2

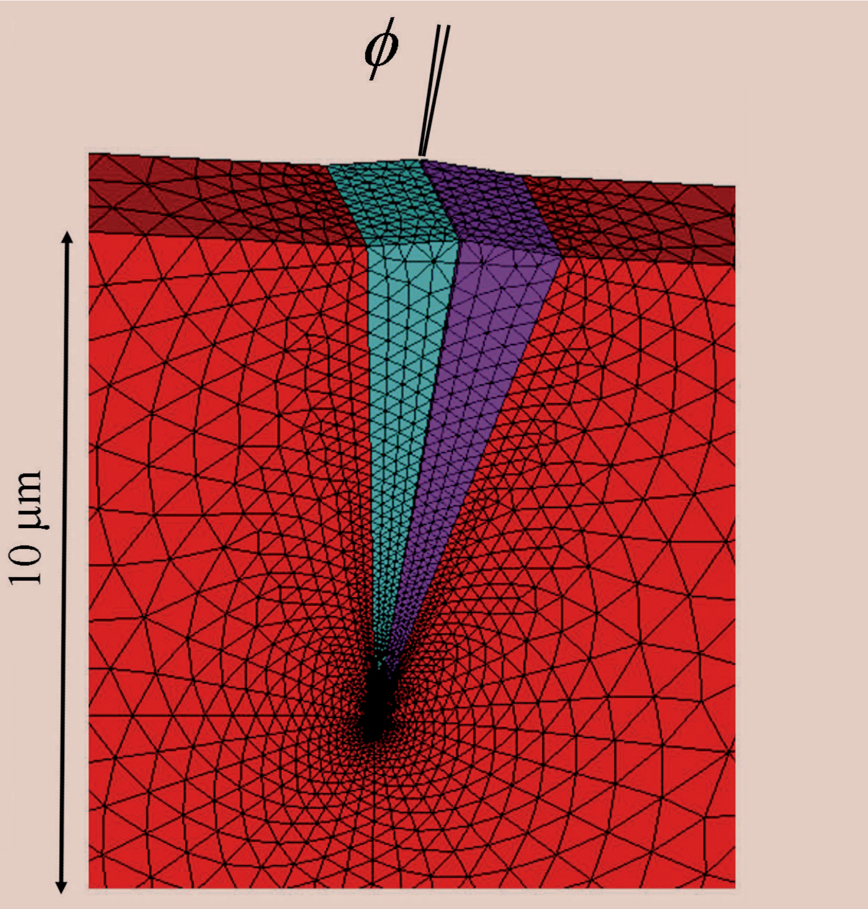
Looking at the symmetry of crystalline solids and the associated consequences. This means investigating the symmetry and kinematics of deformable crystalline solids and studying the implications for the prediction of new stable structures of crystals. This is particularly relevant in terms of assessing explicit constitutive equations for multiphase crystalline materials, for controlling microstructure morphology, and for testing the data found on possible relations in tailor-made crystals.

This RO centres on detailed investigation of the symmetry properties of crystalline materials and their consequences, both in simplified models based on the concept of a simple Bravais lattice and within the more detailed framework of 'multi-lattices'. The main method for symmetry investigation in this context is given by 'Arithmetic Crystallography', this produces explicit criteria for the systematic enumeration of all possible periodic crystal structures which means it can generate complete structure databases. This is a topic of considerable interest, as theoretical structure databases are expected to become a cornerstone of materials science in the future. When coupled with efficient ab-initio methods, they can be mined to produce a host of new theory based stable structures for crystalline materials. Furthermore, this RO also involves detailed investigation of the microstructure in multiphase crystals, something which strongly affects their macroscopic behaviour.

RO 3

We are aiming to develop new tools and concepts for the modelling and mathematical analysis of multiscale problems. We plan to develop and apply advanced mathematical tools for multi-scale problems in phase transformations, as well as to engage in experimental testing of the resulting concepts.

The goal of this RO is to develop and



Analysis of a stressed wedge in a cubic-monoclinic CuZnAl shape-memory alloy

apply new, general mathematical methods for those multiscale problems which arise in phase transitions. In this situation the effective two-way interaction between experimental groups facilitated by the MULTIMAT project comes into its own. On the one hand experimental observations provide the stimulus for the mathematical analysis, on the other new mathematical predictions and possible design criteria for new materials are tested by the experimental groups. The current mathematical theory is extremely advanced with regards to those minimisation problems without internal length scales. Theories which also involve a small, internal length scale are necessary in order to study details of the geometry of the microstructure – this could mean twin branching or the development and interaction of topological singularities in thin magnetic films. It should also be considered that mathematical tools to capture the transition between atomistic and continuum models are still in their infancy. In the context of phase transformation, the phase-field modelling is applied largely because of the ease with which it incorporates the strain-induced long-range elastic interactions generated by the lattice misfits into the formalism.

RO 4

The fourth research objective focuses on computation. The MULTIMAT project aims to develop an innovative method of computer modelling based on appropriate combinations of atomistic and continuum approaches and comparison with experimental data.

In this RO the aim is to compute effective parameters like lattice parameters, bulk moduli and elastic constants, but also to perform mathematical and numerical analysis of such coupled simulations in order to validate the existing methods, to clarify their range of validity, or to propose new numerical approaches. There are strong ties between activities in RO 1 – where quantitative measurements provide input data for these numerical simulations – and RO 3, particularly with regards to bridging the gap between atomistic and continuum modelling. ★

At a glance

MULTIMAT

Objectives:
To improve our fundamental understanding of the underlying principles of the phase transformations which occur in smart materials.

Project Partners:
University of Antwerp, Belgium; Max Planck Institute, Leipzig, Germany; University of Oxford, UK; University of Padova, Italy; Ecole Polytechnique, Paris, France; University of Cambridge, UK; University of Barcelona, Spain; CNRS-ONERA, Châtillon, France; Rheinische Friedrich-Wilhelms University, Bonn, Germany; Academy of Sciences, Prague, Czech Republic; University of Minnesota, US; University of Glasgow, UK.

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