

DEVELOPMENTS IN SOLID MECHANICS AND MATERIALS SCIENCES

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Report from the Organisers:

K. Bhattacharya (Caltech) , P. Suquet, (LMA, Marseille) J.R. Willis (DAMTP, Cambridge)

Virtually every solid material contains features that are different at different length scales. For example, even the simplest piece of metal is made up of many crystallites (grains), which in turn are made up of many atoms. This complexity is compounded in sophisticated modern materials. The microscopic structure of a solid material influences its macroscopic response to applied stress, magnetic field and other macroscopic stimuli. Conversely, the macroscopic applied loads and fields affect the microscopic structure. Microscopic damage may occur, leading ultimately to the formation of large cracks and structural failure. Phase transformations occur in some materials, creating structures at various length scales which evolve with stress.

The challenge, both for mathematics and physical modelling, is to comprehend relationships between models at different length scales. This has led already to a well-developed theory of "homogenization" when the scales are widely separated, and has both exploited and stimulated advances in the calculus of variations. When the scales are separated but still comparable, there is a need for a micromechanical rationale for including scale effects in macroscopic models. The phenomena may be unstable, at least at the microscopic level, and, even if stable, may admit multiple equilibria. Study of the kinetics of the processes is a key requirement, making demands both for modelling and for the analysis of partial differential equations. In particular, the (possibly hierarchical) development of large-scale patterns is an open problem.

The four month programme focused on microstructure, its formation and evolution, and the influence of microstructure on macroscopic properties in the context of phase transformations, damage development and fracture. It brought together specialists in these subjects from diverse disciplines including mathematics, materials science, engineering and physics. It thus provided a forum for the exchange of ideas (both between subjects and disciplines), and facilitated the identification of common issues and exploitation to mutual advantage of the advances in the different areas.

There were three periods of organized activities, an EC summer school and concentration, and two workshops. These consisted of detailed talks (of one hour or longer) with plenty of time for discussion. These periods attracted increased levels of visitors. Smaller groups were in residence during the rest of the programme engaged in detailed collaboration, seminars, tutorials and exchange of ideas.

EC Summer school and concentration on Microstructure and Phase Transformations in Solids

The programme started with a two-week EC summer school on the mathematical developments in modelling microstructure and phase transformations in solids. Recently there have been some exciting advances in developing a mathematical framework for charactering microstructure, and for understanding the link between microstructure and macroscopic properties. These developments were introduced in four expository series of lectures during the first week. The four series dealt with (i) homogenization theory which describes the effective properties when there is a wide separation of scales, (ii) the hierarchy of atomistic models of solids starting from ab initio quantum mechanical methods based on density functional theory all the way to empirical potentials, (iii) the multitude of defects or failure mechanisms in solids including dislocations, damage and fracture and the array of models that describe them, and finally (iv) the mathematical methods for describing and analyzing microstructure and understanding how they arise in phase transforming solids.

The second week of the EC workshop was devoted to detailed lectures on current research activities. There is a mature, though incomplete, understanding of equilibrium microstructures in phase-transforming solids based on models with non-convex energy and results in the calculus of variations. Some talks reported interesting applications of this theoretical framework, while others discussed open questions surrounding the notion of 'quasiconvexity'. Much less is understood about the evolution of the microstructure, and this was addressed at some length in various lectures. A few talks reflected the recent interest in thin films: they dealt with the morphology and defect structure of epitaxial films of electronic materials, and the microstructure of films of active materials with an eye towards microactuators. Methods for understanding the effective behavior of

nonlinear heterogeneous solids, and for obtaining a combined atomic-continuum description were also discussed. Finally, two talks described how many of these ideas have led to the development of real materials. The final two days of the EC workshop was held jointly with the annual meeting of the European (TMR) network on 'Phase transitions in crystalline solids'. The network annual meeting continued for an extra day and a half which was open to EC summer school participants and during which over 25 scientists gave short talks describing their current research.

The EC summer school was followed by a concentration week during which many experts were in residence in the Newton Institute. There were a few lectures held in an informal style, but many more smaller discussions on emerging ideas. A topic which received much attention during this week was the extension of the methods of statistical mechanics to studying the highly correlated microstructure of phase transforming solids.

Speakers during the EC summer school: G. Allaire, M. Finnis, E. Van der Giessen and S. Müller gave the introductory lectures. R.D. James, M. Ortiz, D. Kinderlehrer, R. Abeyaratne, V. Nesi, M.B. Luskin, L-Q. Chen, T.A. Abinandanan, H.K.D.H. Bhadeshia, P. Ponte Castañeda, M. Berveiller, P.H. Leo, B. Spencer, K. Bhattacharya, E.K.H. Salje, G. Friesecke, A.P. Sutton, M. Pitteri, D. Schryvers, J.M. Ball, A. DeSimone and B. Kirchheim.

Speakers during the concentration: L.B. Freund, M. Rao, S. Sengupta, O.B. Naimark, V.P. Smyshlyaev, G.W. Milton, A.P. Sutton.

Workshop on Defect Mechanics and Non-locality

This workshop explored the world of defects at several different scales. Special attention has been paid to homogenisation methods which not only allow for passing from one scale to another, but also could make allowance at any given scale for detail at an adjacent scale.

There are experimental observations which, to be understood, require such interactions between scales, often in the form of characteristic lengths. Formation of patterns of a given size in evolving microstructures, grain size effects in polycrystalline materials, influence of the underlying lattice to understand the Nabarro-Peierls stress, size effects observed in the nonlinear range, provide a few examples of such situations. Another complementary motivation for coupling scales comes from the numerics. It is indeed a common observation that in the framework of classical models, strain or damage can localise in bands of arbitrarily vanishing width which makes the computations extremely sensitive to mesh size and orientation. All these observations have motivated the introduction of "non-local" terms, primarily to explain patterns or to stabilize the numerics, though with an underlying assumption that such terms {it really do} represent the physics. It is believed that these strain-gradients account for the fact that there is no strict separation of length scales between the micro- and macro- structure. However attempts to derive rational theories from microscopic considerations by expanding and truncating fields at the desired order almost inevitably give rise to ill-posed problems.

Experimental motivations, numerical approaches, and theoretical foundations of a rationale for these higher order effects have been presented during the workshop. Some of the results were obtained just before or even during the workshop, showing the timeliness of the topic and the extent of work to be done, for which the workshop has provided directions. One example of the many discussions which arose is the stabilising or destabilising effect of higher-order terms which is still a hotly debated question.

The speakers were: E Aifantis, Y Brechet, JL Chaboche, SJ Chapman, N Fleck, GA Francfort, M Frémond, Y Huang, RD James, R. Luciano, RS MacKay, AB Movchan, O Naimark, A Needleman, GP Parry, P Ponte Castañeda, V Smyshlyaev, C Stolz, N Triantafyllidis, JR Willis, V. Zhikov.

Workshop on Models of Fracture

This workshop concentrated on problems of fracture which are at present being approached by specialists other than engineers, although the problems are of concern to the latter group as well. The community of physicists interested in a range of nonlinear phenomena (from experimental and theoretical viewpoints) was represented, and questions relating to the stability of propagating cracks were extensively discussed, mainly between this group and the engineers and applied mathematicians. Perhaps the most novel and exciting development is the recognition of "crack front waves" and the role that these play in phenomena such as the development of crack front disorder. Direct computational modelling is now possible, employing finite elements linked across each element boundary by cohesive forces. Such modelling yields very specific results of great complexity, and efforts are being made by certain pure mathematicians to model systems of this type employing the tools of homogenization. Allowance for the development of microcracks throughout the medium requires the use of functions of bounded variation and introduces a significant new component in the asymptotic analysis. Some promising results have been obtained for a one-dimensional idealisation, for which it has been shown that the "Cantor" contribution to the variation is not required, thus restricting consideration to the space SBV. Current research is directed towards two and three dimensions. New ideas are needed, and access to guidance from the engineering community about what assumptions may be realistic is one of the by-products of the workshop.

The speakers were: K B Broberg, L B Freund, J R Rice, F Lund, Y Brechet, M Adda-Bedia, H Nakanishi, J-B Leblond, G Dal Maso, G A Francfort, M Falk, J Sivaloganathan, A Braides, G Buttazzo, E Sharon, E Ching, V

Kovtunenکو, L Truskinovsky, K Ranjith, L I Slepyan, W J Drugan, A B Movchan, R Craster, J R Willis, V Shenoy.

Outcome and Achievements

The immediate outcome of the programme is that participants have made new contacts, across disciplinary divides that previously had not been bridged so explicitly and deliberately: interactions which are likely to last into the future have been established between rigorous mathematicians with expertise in the homogenization of partial differential equations with rapidly varying coefficients, engineers concerned with modelling the development of damage during service of materials, and physicists who approach the modelling of materials from an atomistic or quantum theoretic standpoint. Seeds have been sown and the full extent of the benefit will be apparent in a year or two, when contacts established during the programme have had the opportunity to mature into productive collaborations. It is not possible to delineate the full range of possibilities here. However, certain activities were already in evidence during the programme; a selection is described below.

Phase transformations. One of the major problems concerning phase transformations is the development of a realistic model of the kinetics of transformation. Almost universally, across disciplines, descriptions based on first-order kinetics are adopted. Even within this framework, there is at present no credible model which would describe, for example, the development of the type of complex microstructure displayed by shape-memory alloys, and even the propagation of a single interface has only been modelled phenomenologically. R.D. James has proposed a more microscopic description in terms of a gradient flow in a "wiggly energy" field. This has the potential, for example, to explain hysteresis. The analysis was performed in a one-dimensional realisation only. Now, Smyshlyaev and James together are trying to develop two- and three-dimensional theory, combining Smyshlyaev's expertise in high-frequency asymptotics acquired through the study of diffraction problems, with James' appreciation of the physics of the process, and the expertise of both in homogenization. Another interaction in the area of phase transformations is between Bhattacharya and Ponte Castañeda. The former has already found estimates of the range of stress-free strain of polycrystalline shape-memory materials, while the latter has developed what is probably the most useful and accurate method for homogenization of a nonlinear composite material. The project is to develop and apply this methodology to obtain further insight into the stress-free strain regime.

Thin films. Thin films of ferroelectric material have potential use as actuators, and also as memory devices. One study, motivated by the latter application, is under way between Bhattacharya, Shenoy (INI participants) and Scott (Cambridge, Earth Sciences). The thin film is sandwiched between metal plates. If the film is too thin, boundary layers usually ignored in modelling the ferroelectric switching occupy a large fraction of the volume of the ferroelectric and compromise the performance. The project is to model the boundary layers so that the limiting thickness can be quantified. Another project, between Bhattacharya, Francfort and Fonseca, is concerned with modelling the decohesion of a thin layer deposited on a substrate, so that it is under stress either through pseudomorphic alignment or through thermal mismatch. If the layer is too thick, decohesion is favoured energetically. Variational methods are being developed, to provide a rigorous bound for critical thickness.

Non-locality. There is at present great interest in non-local models, which may describe the deformation of a material with microstructure in the case that the scale of the macroscopic variation is greater than that of the microstructure, but not so much greater that the homogenization limit applies. There are many phenomenological models of unproven validity, a few models based on analysis of micromechanisms, and virtually no rigorous theory. One promising interaction is between Frémond and Zhikov, which will address the modelling of media with extensive ties which link distant particles. Their approach will make use of Zhikov's recent development of homogenization in terms of measures. Analysis at the less rigorous level associated with mechanics is being pursued by Drugan, Luciano and Willis in the context of randomly inhomogeneous media (there is more precise related work by Smyshlyaev and Cherednichenko in the simpler context of media with periodic microstructure). This research has led to explicit non-local constitutive relations which cannot be quantified exactly but whose operators can be bounded in Fourier transform space. Gradient approximations follow from small wavenumber expansions. There is at present a real difficulty in determining the range of validity of these gradient approximations. There is also a difficulty in determining in advance which gradient formulation (if any) will lead to a well-posed problem. Such questions, together with related concerns for identifying boundary conditions that are physically correct as opposed to mathematically convenient, have major implications for the modelling of the development of damage (growth of voids or microcracks during service). There is already quite a major industry of including non-locality into finite element codes, with parameters chosen so as to smooth out localization of deformation. The research in progress will assist in identifying when such smoothing is a physically realistic phenomenon and when it has simply the status of a mathematical device.

Fracture. The programme stimulated interactions between mathematicians, engineers and physicists interested in fracture problems. One such interaction involves Movchan, Rice, Sharon and Willis. Rice observed by

computation a new type of wave, a "crack front wave", that propagates without attenuation or dispersion along the front of a propagating crack. Its existence has been confirmed analytically from a solution of Movchan and Willis, and experimentally by Sharon. Two aspects are under further development: Movchan and Willis are investigating the influence of viscoelastic dissipation (already seen in experiments of Sharon on PMMA), and Rice and Willis are investigating whether crack front waves can exist under conditions of shear loading, as occurs during an earthquake.

[Back to Top](#)

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