EUROPEAN MECHANICS SOCIETY

Colloquium Final Report

N. 601 – Micromechanics of Defects in Crystalline Solids and Metals

Dates and location: **11/06/2018 - 15/06/2018, Sevilla, Spain**

Chairperson **Pilar Ariza**

Co-Chairperson **Viggo Tvergaard and Michael Ortiz**

Conference fees

- Regular registration fee **500.0 €**
- Accompanying person registration fee **150.0 €**

What other funding was obtained? **We have received financial support from the University of Seville, through the program VI Plan Propio de Investigación y Transferencia de la US, year 2018.**

What were the participants offered? **The registration fees indluded:**
- The book of abstracts.
- Visit to Hospital de la Caridad and Welcoming cocktail-dinner.
- 2 daily coffee breaks and five lunches.
- Excursion to visit the city of Cádiz and the gala dinner at Venta de Vargas in San Fernando (Cádiz).

Number of members of Euromech (reduced registration fee) **16**

Number of non-members of Euromech (full registration fee) **31**

Applicants (members)

- Pilar Ariza
- William Curtin
- Dennis Kochmann
- Varvara Kouznetsova
- Jean-Baptiste Leblond
- Dominique Leguillon
- Javier LLorca
- Alan Needleman
- Pedro Ponte-Castaneda
- Daniel Rittel
- Massimo Ruzzene
- Claude Stolz
- Stanislaw Stupkiewicz
- Bob Svendesn

- Viggo Tvergaard
- Kerstin Weinberg

Applicants (non members)

- Amit Acharya
- Eleni Agiasofitou
- Francisco Arca Cebrián
- Gustavo Castelluccio
- Héctor Cifuentes
- Sergio Conti
- Vikram Deshpande
- Jose Fernández-Sáez
- Vikram Gavini
- Ercan Gürses
- Stefanie Heyden
- Henrik Myhre Jensen
- Markus Lazar
- Mathias Lebihain
- Brian Nyvang Legarth
- Mitchell Luskin
- Jaime Marian
- Xanthippi Markenscoff
- Emilio Martínez-Pañeda
- Juan Pedro Mendez Granado
- Alain Molinari
- Alejandro Mota
- Michael Ortiz
- Mauricio Ponga
- Javier Ramos
- Jose David Rios Jimenez
- José Rodríguez-Martínez
- OUADIE SABRI
- Pratheek Shanthraj
- Haiyang Yu
- Ramon Zaera-Polo

Scientific Report

Recent developments in experimental science that enable the examination of defects at the atomic scale provide an unprecedented connection between the structure and properties of materials. Techniques ranging from high-resolution electron microscopy to atomic-force microscopy reveal new insights into the micromechanical foundations of material behavior, but also pose deep challenges as regards theory, modeling and simulation. However, the link between the defects themselves and the observed macroscopic behavior is often a difficult one to forge theoretically or computationally and remains an active area of research. Many of the fundamental mechanisms underlying the inelastic behavior and failure of materials are mediated by crystal-lattice defects and are, therefore, accessible to direct atomistic simulation, either by means of empirical potentials or through ab initio quantum-mechanical calculations. Notable examples are furnished by first-principles calculations of the EoS and elastic moduli of metals up to high pressures and temperatures, and the characterization of the structure of point defects, such as vacancies and interstitials, and extended defects, such as dislocations, grain boundaries and cracks. However, in general atomic-scale mechanisms are separated from macroscopic behavior by a vast array of intervening continuum

scales. These mesoscopic scales both average and set the boundary conditions or driving forces for the atomic-scale phenomena and are an essential part of the structure of materials. While effective at describing macroscopic material behavior, continuum theories tend to break down on the scale of the lattice, e. g., in the vicinity of lattice defects. Therefore, a complete understanding of material behavior and failure, as well as the predictive computation of the material properties, requires both atomistic and continuum modeling, with the atomistic/continuum handshake most effectively achieved within the framework of multiscale modeling. The goal of the EUROMECH colloquium 601 was to bring together a diverse group of researchers from various areas ranging from theoretical, experimental and computational modeling of the mechanics of materials.
Altogether there were 47 participants and 39 presentations. The list of participants and the full programme are available in a separate document. Most importantly, there was ample time for informal discussions among the participants during coffee breaks, lunches and social activities.
Specific topics addressed in the talks and discussed included:
• Elastic defects and configurational forces
The closed?form expressions of the J?, M?, and L?integrals between two straight (edge and screw) dislocations were discussed in the framework of three? dimensional, linear, incompatible elasticity theory. The J?integral of dislocations is the well?known Peach?Koehler force (interaction force) between two dislocations. The derived results provide a new insight into the physical interpretation of the M?, and L? integrals of dislocations.
• Effective/homogenized properties of composites
Constitutive models for the finite?strain, macroscopic response of porous viscoplastic polycrystals, bounding global behavior for composite with an imperfect interface between phases and the role of micro?inertia effects in the overall response of heterogeneous materials were discussed extensively during the colloquium. New improved bounds were presented and demonstrated in a number of areas of application.
• Mixed continuum/atomistic/DFT models
For accurate modeling of polycrystalline metals, it is essential to understand the dislocation?based mechanisms that control the plastic flow on the different slip systems in metal alloys. Current approaches fit standard crystal plasticity models to experimental data, which implicitly assumes all plasticity to occur by normal glide and hardening mechanisms. A theory for the cross?slip energy barrier was presented, with first?principles density functional theory (DFT) calculations used to compute the necessary pyramidal stacking fault energies as a function of solute type for many solutes in the dilute concentration limit.
• Diffusive molecular dynamics and mass transport
Dislocation?solute interactions are at the heart of many important processes in materials science and metallurgy, such as solid solution strengthening, dynamic strain ageing, pipe diffusion, etc. This interaction is complex, and can result in material softening and/or hardening depending on temperature and solute concentration. The subject was the focus of a number of presentations and of extensive discussion. A kinetic Monte Carlo approach to the coupled transport problem in three dimensions was presented. Moreover, a novel framework capable of retaining full atomistic resolution while simultaneously enabling the simulations of long?term mass transport was applied to study the electric charge process in Si? based anode Li batteries, in which Li cations enter and diffuse into the Si lattice, and as a consequence Si anode loses its crystalline structure and the alloy becomes amorphous, with a considerable volume increase. Furthermore, a new technique was introduced for enhanced free?energy sampling and accelerated dynamics in atomic systems. This new technique is based on the concept of coarse?grained dynamics or mesodynamics and temperature acceleration of rare events. The system is evolved using averaged positions and momenta that are

computed using a probability density function at some relevant temperature of interest.By so doing, it is possible to demonstrate that the phase averaged forces felt by the atoms are directly related to the free?energy of the system at the temperature of interest. This relation was exploited and used to perform accelerated mesodynamics of atomic systems by recourse of temperature acceleration.

• Two-dimensional/multifunctional materials

Metamaterials have gained import thanks to recent advances in small?scale fabrication techniques. Among the sought-after target properties are typically high stiffness?to?density and strength?to?density ratios. Periodic truss networks have attracted particular attention, owing to their simple design principles and the achievable high stiffness and strength as well as energy absorption and recoverability. Different type of periodic metamaterial whose anisotropic elastic properties can be tailored similarly to nanotruss networks but whose strength and recoverability are significantly superior were presented and discussed. Also, a novel approach for calculating the mechanical relaxation pattern of incommensurate bilayers over configuration space, bypassing the need for the standard supercell approximation and giving a true aperiodic structure was introduced. The model can be used for a wide variety of materials via use of a continuum model for intralayer interactions and the generalized stacking fault energy for interlayer interactions.

• Dislocation dynamics and crystal plasticity

During the meeting, a method for solving small strain plasticity problems with plastic deformation arising from the evolution of a collection of discrete shear transformation zones (STZs) was presented. The formulation is analogous to that for discrete dislocation plasticity. The shear transformation zones (STZs), the carriers of plastic deformation, were modeled as Eshelby inclusions. Superposition was used to represent a quasi?static boundary value problem solution in terms of: (i) discretely modeled Eshelby inclusions, given analytically for an infinite elastic medium; and (ii) an image solution that enforces the prescribed boundary conditions. Results for various boundary value problems and for various constitutive characterizations of STZ kinetics were presented. Moreover, a new approximation scheme for three?dimensional dislocation dynamics in which the dislocation density is concentrated at points, or monopoles, was presented for the first time at the colloquium. The monopoles move according to mobility kinetics driven by elastic and applied forces. The fundamental difference with traditional approximation schemes based on segments is that in the proposed approach an explicit linear connectivity, or 'sequence', between the monopoles need not be defined. The monopoles instead move as an unstructured point set subject to the weak divergence constraint. In this sense, the proposed paradigm is 'line?free', i.e., it does not require the tracking of dislocation lines. This attribute of the formulation offers significant computational advantages in terms of simplicity and efficiency.

• Multiscale modeling and simulation of polycrystals

The recently developed iterated second?order homogenization method for porous polycrystals consisting of large pores randomly distributed in a fine?grained polycrystalline matrix was applied for the development of constitutive models for the finite?strain, macroscopic response of porous viscoplastic polycrystals. The method makes use of a linear comparison composite (LCC) with the same substructure as the actual nonlinear composite, but whose local properties are chosen optimally via a suitably designed variational statement. The approach can be used to generate estimates for both the instantaneous effective response and the evolution of the microstructure for porous FCC and HCP polycrystals and single crystals under various loading conditions.

• Multiscale models of microstructure evolution

Collective dislocation behavior in metallic systems is highly dissipative in nature and results in the formation and evolution of a wide variety of microstructures.

Discrete modeling approaches for this at the mesoscopic level include for example kinetic Monte Carlo or line dislocation dynamics. In particular, the use of coarse?graining of dislocation dynamics in the context of non?equilibrium statistical thermodynamics with the help of projection?operator and fluctuation?dissipation methods as well as the General Equation for Non? Equilibrium Reversible Irreversible Coupling (GENERIC) was discussed. Moreover, a multiscale modelling roadmap was presented to study precipitation hardening in Al?Cu alloys. In the first step, the homogeneous and heterogeneous formation of precipitates during high temperature ageing in Al?Cu alloys is simulated using the phase?field model in which the model parameters that determine the different energy contributions (chemical free energy, interfacial energy, lattice parameters, elastic constants) were obtained from either computational thermodynamics databases or from first?principles density functional theory. From the information, the evolution and equilibrium morphology of precipitates in 3D was obtained. The new methodology to study the dislocation/precipitate interactions opens the possibility to obtain quantitative estimates of the strengthening provided by precipitates in metallic alloys using multiscale modelling strategies based on first principles calculations.

• Multiscale/regularized models of brittle damage/fracture

While cracks are actually sharp two? dimensional hypersurfaces, the use of a continuous order parameter field ?or phase field? regularizes the sharp material discontinuities with smooth transitions between broken and unbroken regions. The scope of a phase?field fracture approach was demonstrated through finite element simulations of brittle fracture in a Brazilian test specimen and its comparison to experimental results. The main challenge of such fracture simulations is that it requires the prediction of crack nucleation and fracture without stress concentration at a notch or at an initial crack.

• Ductile fracture and crazing

One of the most common mechanism of ductile fracture for metals is the nucleation, growth and coalescence of micro?voids. A multiscale modelling of dynamic failure allowing to elucidate the role of micro?inertia effects in the fracture process was presented during the meeting. For large volume fractions of voids ahead of the blunted crack?tip multiple voids will grow simultaneously. On the other hand, only one void expands at a time and coalesces with the crack?tip for small void volume fractions. General orientations of the anisotropy relative to the crack?plane within a plane strain setting accounting for finite strains were discussed and applied to a plastically anisotropic aluminum Al 2090?T3 model. Moreover, a cell model analysis was presented to study the nucleation and subsequent growth of voids from a non?uniform distribution of inclusions in a ductile material. Nucleation was modeled as either stress controlled or strain controlled. The special clusters considered consist of a number of uniformly spaced inclusions located along a plane perpendicular to the maximum principal tensile stress. After nucleation, local void coalescence inside the clusters was accounted for, since this makes it possible to compare the rate of growth of the single larger void that results from coalescence in the different clusters. Nucleation parameters leading to rather early nucleation, or to later nucleation, were considered.

• Multiscale modeling of cell/tissue mechanics

One area of tremendous societal impact where mechanics, both theoretical and computational, can make game-changing contributions is medical engineering. This potential for disruptive contributions was exemplified during the meeting, by means of a recently developed mathematical model of information transmission across the biological neural network of the human brain. The overall function of the brain consists of the emergent processes resulting from the spread of information through the neural network. The capacity of the brain is therefore related to the rate at which it can transmit information through the neural network. The particular transmission model allows for information to be transmitted along multiple paths

between points of the cortex. The resulting transmission rates are governed by potential theory. According to this theory, the brain has preferred and quantized transmission modes that correspond to eigenfunctions of the classical Steklov eigenvalue problem, with the reciprocal eigenvalues quantifying the corresponding transmission rates. These findings have immediate implications for testing the hypothesis that the sulcus pattern of the human brain has evolved to maximize the rate of transmission of information between points in the cerebral cortex, and for potential clinical applications including epilepsy and drug-resistant depression.

• Continuum thermodynamics models of inelasticity

Dislocations and their interaction with precipitates and alloying chemistry are critical mechanisms that play a central role in the design of complex materials. In presentations, atomistic phase?field microelasticity (APFM) was shown to predict dislocation core structures. The results were compared directly with molecular dynamics (MD) simulations for the model system of Ni? Ni3Al, and the formation of anti?phase boundary and complex stacking faults inside the Ni3Al precipitate were observed to be in good agreement with the MD results. Furthermore, the APFM was coupled with a thermodynamics?based model for solute transport, and the coupled dislocation?solute problem was benchmarked for the Ni?Al?Co system.

We thank Euromech and the University of Seville, especially the Engineering School, for making the meeting possible and for financial and organizational support.

Number of participants from each country

Country	Participants
Germany	7
Spain	10
United States	11
Denmark	3
Switzerland	2
France	5
United Kingdom	4
Poland	1
Canada	1
Israel	1
Netherlands	1
Turkey	1
Total	**47**

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