EUROMECH COLLOQUIUM 653
International Colloquium on Mechanics of Interfaces

August 26th-28th 2025, Metz, France

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Disconnection flow-mediated microstructure evolution

Marco Salvalaglio[1], Caihao Qiu[2], Jian Han[2], David J. Srolovitz[3]

The evolution of polycrystalline microstructures is primarily governed by the migration of grain boundaries (GBs), which separate individual crystalline grains of different orientations. This migration is fundamentally mediated by the motion of line defects, known as disconnections, which propagate along the GBs and possess both step and dislocation characters. This presentation illustrates recent findings on how disconnection flow influences microstructural evolution.

Using a bicrystallography-consistent continuum model [1], we first discuss key phenomena associated with disconnection-mediated GB motion, such as GB faceting and grain rotation [2]. Then, through a phase-field formulation of this model, we demonstrate that internal stresses generated by disconnection flow (shear coupling) induce significant deviations from classical curvature-driven grain growth in microstructures. These deviations match well with recent experimental observations, which indicate a lack of correlation between GB velocity and curvature in polycrystals, an effect that conventional models fail to capture [3].

We conclude by discussing that a thorough description of GB motion requires not only accounting for internal (and external) stress contributions but also redefining the concept of GB mobility. Atomistic simulations, analyzed using a Markov chain model, reveal that asymmetric GBs exhibit direction-dependent velocities due to differing disconnection nucleation barriers on their opposite sides [4]. Consequently, mobility is not just a proportionality constant between GB velocity and driving force. Such evidence implies that oscillatory driving forces or cyclic thermal annealing can induce unidirectional motion of asymmetric GBs, akin to Brownian ratchets [4]. We also briefly outline experimental confirmations for this behavior and implications for accelerated grain coarsening in microstructures upon oscillating driving forces.

Keywords: Disconnections, Grain Boundaries, Microstructures, Continuum Modeling

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Quantification of the grain boundary structure and determination of migration mechanisms

Luis A. Barrales-Mora[1], Gashaw Bizana[2]

Grain boundary migration has been investigated for several decades. It is accepted that a grain boundary can move under the action of mechanical stresses and jumps in chemical potential [1, 2]. A jump in chemical potential occurs whenever there is gradient of any intensive thermodynamic variable for example grain boundary curvature. Experiments and simulations have substantiated differences in the motion of grain boundaries depending on the acting driving force [3-6]. Different activation enthalpies have been determined to be different for crystallographically similar grain boundaries. The migration enthalpy is a fingerprint of the migration mechanisms, which in turn depends on the grain boundary structure. In the present contribution, persistent homology (PH) was utilized to quantify the structure of the grain boundaries during their migration. To this aim, more than 1200 MD simulations of GB migration were performed. In these simulations, mechanical stresses and a jump in chemical potential were used to drive the motion of the boundaries. We show that PH can be used to quantify the GB structure and that by association it is possible to discriminate the type of migration of a boundary.

Keywords: Grain boundary migration, shear driven motion, persistent homology, chemical potential driving force

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Plastic displacement as a collective variable to study shear-coupled grain boundary migration and grain boundary phase transitions

Nicolas Combe[1,2], Frédérique Mompiou[1,2], Mar Legros[1,2]

In absence of dislocation activity, grain boundary(GB) migration can operate as an efficient vector of plasticity. The shear coupled grain boundary migration (SCGBM) mechanism has focused a peculiar attention due to its conservative nature and ability to operate at low temperature. Nucleation and motion of disconnections constitute the elementary mechanisms of the GB migration[1-3]. Using atomistic models, the nudge elastic band method has revealed to be a powerful tool to quantitatively characterize the disconnection properties[4-6]. However, this method only operates at 0 K which significantly limits the comparison of its results with experimental data. Furthermore, this restriction strongly limits the investigation of temperature-activated SCGBM modes or the migration of GB whose structure varies with temperature.
We propose in this work to use the plastic displacement as a collective variable in order to compute the free energy barrier for the SCGBM at different temperatures[7]. This method allows to account for entropic effects during the migration. Performing a commitor analysis, the plastic displacement constitutes a relevant reaction coordinate to study SCGBM. Furthermore, we demonstrate that the temperature induced GB transition phases may be examined and characterized thanks to this novel approach.

Keywords: Grain boundaries, disconnections, free energy, grain boundary phase transition

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Relating Grain Boundary Structure to Dislocation Models

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Many grain boundaries can be modeled as arrays of interfacial line defects such as dislocations and interfacial steps, or, more generally, disconnections (i.e., interfacial steps that also possess dislocation content). Such models are useful because they provide insights into the properties and behavior of grain boundaries in terms of the individual unit behaviors and interactions of the defects. Often, the defects at high angle grain boundaries are defined with respect to bicrystalline reference states that typically possess low CSL values and often correspond to local minima in the energy of the boundary as a function of misorientation or inclination. However, it can also be useful to consider the structure of boundaries in terms of dislocations defined with respect to a single crystal reference state. This is very much the case at boundaries in FCC metals for which the tendency to maintain close-packing is well captured by models for which the interface is composed of arrays of full and partial crystal dislocations.

We illustrate these ideas in this presentation, drawing on examples from our atomic resolution electron microscopic observations and atomistic simulations of FCC grain boundaries and their defects. We discuss first the classic example of Σ3 {112} grain-boundary facets, which are well described as dense arrays of Shockley partial dislocations. We then extend this model to analyze how these dislocations must be arranged at grain boundary facet junctions. We find that such junctions constrain the sequence of dislocations that can allow for motion of the junctions through coordinated, conservative glide, a result we investigate with complementary molecular-dynamics simulations. A key result is that for some configurations of facets, topological constraints require the formation of $\frac{a}{2}\langle 110\rangle$ unit jogs. Because the unit jogs require the absorption or emission of point defects to move, they will limit the motion of the junctions. Another manifestation of Shockley partial dislocations at boundaries in metals with low stacking fault energies is the dissociation into 3D interfacial configurations composed of densely spaced stacking faults. Here, we investigate such dissociation at boundaries vicinal to Σ33a, which dissociate into a narrow band of 9R stacking (... abc/bca/cab ...). Remarkably, this dissociation only occurs for a narrow angular range of boundary inclinations. As we discuss, the strong dependence on boundary inclination can be well understood and related to other dissociated boundary structures by modeling the necessary arrangements of lattice dislocations required to accommodate the misorientation and inclination. *SNL is managed and operated by NTESS under DOE NNSA contract DE-NA000352.*

Keywords: Grain boundaries; Interfaces, Dislocations; Facet Junctions

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Stress-induced amorphization and grain-boundary sliding

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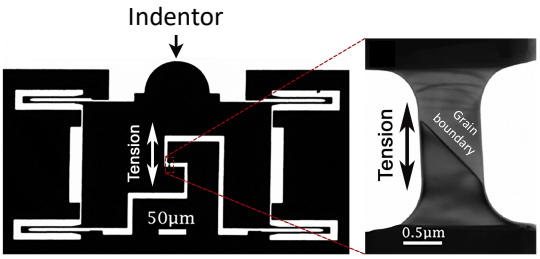
Stress-induced amorphization has recently attracted attention as a potential deformation mechanism in ceramics, semi-conductors or minerals [1]. Its activation is promoted when conventional plasticity, *e.g.* driven by dislocations, is inhibited, however the underlying mechanisms are still unclear. In this study, we focus on olivine, a magnesium-iron silicate that is a major constituent of the Earth's upper mantle. Using quantitative *in situ* TEM tensile testing, we demonstrate that stress-induced amorphization can be activated under high stresses at room temperature in small-sized olivine bi-crystals. High-angle grain boundaries are the preferred sites for amorphization whereas low-angle grain boundaries are less prone to this phenomenon. Amorphized grain boundaries are then subject to sliding and the resulting constitutive equation of such a sliding boundary has been determined. We show by Molecular Dynamics that this phenomenon can be considered as a case of transformation plasticity. Varying the iron content in olivine demonstrates that iron inhibits amorphization and, consequently, promotes brittle failure. This is in contrast to the accepted view at high temperatures where iron promotes ductility in olivine. These findings coming from natural minerals provide a novel approach to the control of the mechanical properties of grain boundaries in hard materials at low temperatures following a geomimetic inspiration.



Keywords: Amorphization, Grain boundary sliding, Transformation plasticity, Olivine

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Micromechanical modelling and atomistic simulations of solute atom segregation towards grain boundaries

Joé Petrazoller[1], Julien Guénolé[1], Stéphane Berbenni[1], Thiebaud Richeton[1]

The mechanical properties of metallic polycrystals are strongly influenced by solute atoms segregation towards grain boundaries. This mechanism can affect several of their properties, such as their energy, cohesion or mobility. A solute atom can be represented by a point force distribution, corresponding to the forces imposed on atoms surrounding the defect. The first order moment of this distribution, named “elastic dipole”, is used to calculate the long-range elastic fields. Using the method described in [1], the permanent elastic dipole, which can be linked to an eigenstrain tensor, and the diaelastic polarizability tensor, which is related to the change of the alloy’s elastic constants, have been determined by atomistic simulations for both Ni and Ag atoms embedded in FCC Ag and Cu matrices, respectively, and for Al and Y atoms embedded in HCP Mg matrix. Following the crystallographic structure, the permanent elastic dipole and polarizability tensors exhibit different shapes. Then, the interaction energy between the elastic dipole and the stress fields of several symmetric tilt grain boundaries have been calculated. The stress fields have been evaluated from the Virial stress fields given by molecular static simulations or from the stress fields of dislocation walls, either in heterogeneous anisotropic elasticity [2] for anisotropic FCC lattices or in isotropic elasticity [3] considering a non-singular continuum theory of dislocations [4] for Mg HCP lattices. The latter has been considered for grain boundaries where the tilt axis is along <c> and <a> directions. Additionally, the segregation energy of a single solute towards a grain boundary has been computed using a series of molecular statics simulations. Comparisons between this segregation energy and the different interaction energies highlight the importance to consider elastic anisotropy for anisotropic materials in order to capture differences between grain boundaries with a same tilt angle [5]. Furthermore, to fully model solute interaction with GB, we highlight the importance to consider, in some situations, the deviatoric stresses of the GB, in addition to the traditionally only considered hydrostatic stress. All these results ultimately help bridge the scale gap to build a continuous-based segregation model similar to that of White and Coghlan [6], incorporating anisotropic elasticity and GB deviatoric stresses, and predicting solute concentration distributions at grain boundaries.

Keywords: Solute segregation, anisotropy, grain boundaries, micromechanical model, molecular statics

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How neighbour interactions influence rheology and grain rotations under Coble creep

Laurent Delannay[1], Saad Mortadi[1], Francis Delannay[1]

This work investigates the viscoplastic deformation of polycrystalline aggregates under the cooperative displacements of adjacent grains. We consider that grain boundary sliding (GBS) is accommodated by grain boundary diffusion (Coble creep) and question the influence of the sizes and irregular shapes of grains on the relative contributions of diffusion and GBS to the average deformation of the aggregate. Whereas the frequently used, unrealistic assumption of an affine displacement field involves equal contributions of both deformation modes, irregular grain samplings are shown to favour GBS. A numerical model is developed with the aim to predict both the macroscopic rheology and the microscopic field of displacements and grain rotations in periodic 2D polycrystals (Fig. 1). Grain rotations are found to depend both on the heterogeneity of grain shapes, and on the microscopic viscous shear stress opposing GBS. Hence, experimental observations of the statistics of grain rotations (and velocity mismatches along GB) constitute valuable information to probe the micromechanical response.

Keywords: grain boundary sliding, diffusion-aided creep, lattice rotations.

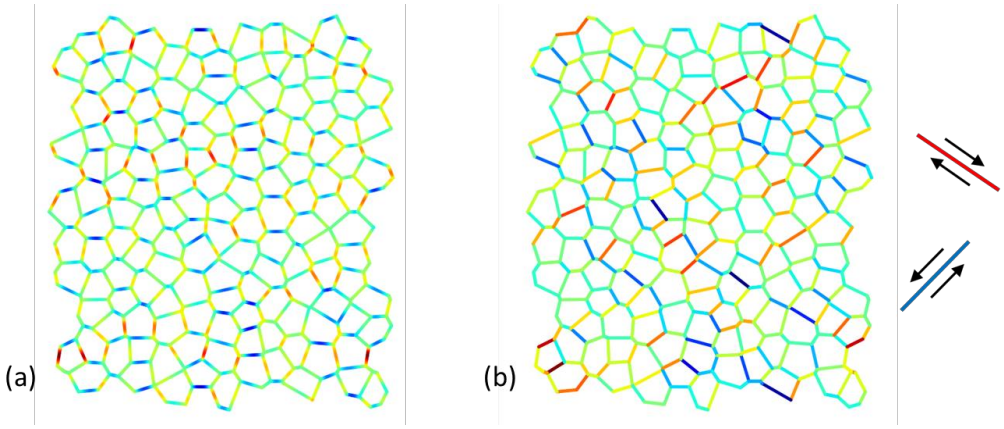

Figure 1: Diffusion-aided GBS inside a polycrystal with irregular grain shapes. (a) The stress normal to the GB is the diffusion potential. (b) The amount of GBS depends on the grain topology.

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Dislocation density fields for bridging length scales in interface-dominated nanomechanics

Julien Guénolé[1], Houssam Kharouji[1], Yen Fred Woguem[1], Vincent Taupin[1]

The nanomechanics of crystalline materials is governed by various processes occurring across a wide range of length/time scales. While continuum mechanics simulations offer a suitable framework for modeling the mechanical properties of microstructures, they are limited in capturing the details of crystal defect structures and their elementary deformation mechanisms. On the other side, these mechanisms can be conveniently accessed through discrete atomistic simulations, but such approaches are usually limited to small length/time scales. Now more than ever, as the boom in simulation resources and methods is combined with the rise of machine learning, accurate information transfer across scales is required for efficient and reliable physics-based plasticity modelling.
The work we present here explores a novel atomistic-to-continuum crossover scheme based on dislocation density fields [1, 2]. More precisely, elastic transformation tensors are computed using the Hartley and Mishin method for atomistic configurations, and then employed as inputs in a micromechanical field dislocation mechanics (FDM) strain-gradient type model using a regular fast Fourier transform solver grid. This versatile approach successfully captured, defects as diverse as dislocations and high-angle grain boundaries, as well as interactions among them (Fig. 1). Assessments of this approach with cubic (Cu, Al) and hexagonal (Mg, Ti) materials is presented. The prediction by means of machine learning approaches of interfaces characteristics as represented by dislocation density fields is also explored. In the light of our results, the implication of such a discrete-to-continuum crossover for bridging scales in nanomechanics is discussed.

Keywords: atomistic, continuum, grain boundary, dislocation.

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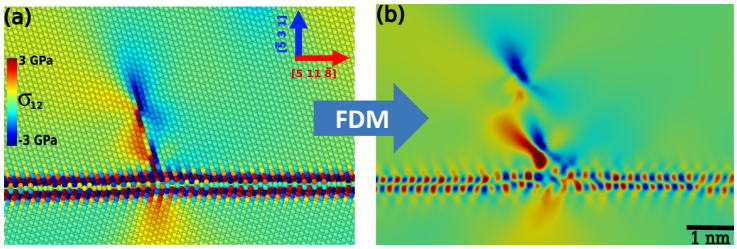

Figure 1: Interaction between an extrinsic edge dislocation and a Σ35(531)[112] 34.05° high angle tilt grain boundary in copper. (a) Per-atom Virial stress σ_{12}. (b) Continuous elastic stress field σ_{12} obtained using the G method.

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Disconnection Mechanics: Segregation, Stability, and Mobility at Interfaces.

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Grain boundaries are ubiquitous features in polycrystalline materials, having an outsized influence on material properties in nanocrystalline metals. Among the crucial features dictating the behavior of these grain boundaries are grain-boundary defects, notably disconnections. Disconnections are peculiar defects that possess both dislocation and steplike characters and impact various grain-boundary properties.
In this talk, I will discuss the atypical properties of disconnections in in binary alloys revealing their pivotal role in dictating solute segregation phenomena at grain boundary and their stability. I will first discuss their role in segregation patterning for a broad range of binary alloys. I will review the root cause of various segregation patterns which are associated break of local symmetry caused by the dislocation content at the step region of the disconnection. The local stress fields associated with different disconnection configurations are fundamental to these phenomena and have been analyzed through both atomistic simulations and continuum-based dislocation-disclination mechanics, revealing a strong correlation between local pressure and segregation behavior [1]. With this understanding of segregation patterning, I will then introduce interfacial defect diagrams, derived from simulations and segregation theory, to predict the stability and mobility of disconnections within the temperature-solute concentration phase space [2]. These diagrams highlight various stability regimes governed by solute-induced clustering and pinning effects that significantly impact the thermal migration of disconnections. Overall, this talk will offer critical insights into the thermodynamics and kinetic properties of interfacial defects and their impact on the properties of nanocrystalline alloys. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

Keywords: segregation; disconnections; dislocations;

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Architectured bi-lattice materials inspired by analogues in bi-crystal plasticity

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Thiebaud RICHETON[1], Justin DIRRENBERGER[3], Stéphane BERBENNI[1]

Additive manufacturing has allowed the development of architectured materials in the industry. However, despite their advantages, such as their low density and good energy absorption, the use of cellular materials as structural components is still hindered by concerns toward their mechanical stability and resistance [1]. In particular, highly periodic stretch-dominated lattice structures are subjected to the emergence of localization bands [2], which causes mechanical instabilities and early structural failure in the plastic regime. A framework for improving the mechanical resistance of those lattice metamaterials consists in drawing from an analogy between the macroscopic lattice structures and the crystalline microstructures to derive design guidelines from crystalline properties to obtain the desired mechanical response in metamaterials [2]. For example, the introduction of defects like interfaces between different lattice orientations has been shown to hinder localization band propagation in an analogous manner to the interaction between grain boundaries and slip bands in polycrystals [2].
The objective is to more thoroughly explore this analogy by applying two approaches, one based on bi-crystallography and the other on crystal plasticity, to design bi-crystal inspired octet-truss lattice structures. The first approach developpes the geometrical analogy by using the crystallographic Coincidence Site Lattice (CSL) theory to obtain various interface morphologies in the bi-crystal inspired structures. This allows to test the influence of specific interfacial connectivity on both local and global mechanical behaviors. Hence, it opens the possibility to tailor the metamaterial's interface for certain applications. The second approach stems from the search for a mechanical analogy between crystalline slip and the metamaterial's localization bands. Since both phenomena drive plastic deformation and occur in preferential planes [3], this approach proposes to adapt an analytical bi-crystalline model [4] in an incremental formulation implemented in a python code. These fast calculations will be used to optimize the bi-crystal inspired truss mechanical response.

Acknowledgements
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Keywords: Architectured Materials, Additive manufacturing, Bi-crystal, Interface.

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Reverse Engineering Grain Growth Kinetics from Time-Resolved 3D Grain Maps and Machine Learning

Jules M. Dake,[1] Helmuth-André Schulz-Harder,[1] Leonard Lauber,[1] Mingyan Wang,[1]
Thomas Wilhelm,[2] Lukas Petrich,[2] Orkun Furat,[2] Haixing Fang,[3] Pierre-Olivier Autran,[3]
Volker Schmidt,[2] Wolfgang Ludwig[3] and **Carl E. Krill III**[1]

Understanding grain growth remains an exceptionally tough nut to crack. Statistically, its evolution appears monotonous—after all, the average grain size changes in only one direction—but at the level of individual grain boundaries (GBs), microstructure evolution is strikingly complex. The variation in local effective GB properties is especially pronounced during the phenomenon of *abnormal grain growth,* where a select few grains outpace those in the surrounding matrix. Although physical factors drive this runaway growth, our understanding remains largely empirical, with no consensus on its mechanistic origins.

Thanks to the advent of x-ray microscopy techniques like diffraction-contrast tomography (DCT), we now have experimental access to the full four-dimensional (3D + time) parameter space of GB migration. Presumably, the mechanisms governing any form of grain growth are encoded in such inherently vast datasets. However, manually extracting parameters like a GB's 'reduced mobility' is both tedious and error-prone [1], while directly fitting numerical grain growth models to experimental data is computationally intensive and fundamentally constrained by model assumptions [2]. This talk will present fresh perspectives on abnormal grain growth derived from time-resolved DCT reconstructions, with microstructural analysis enhanced by a convolutional neural network utilized to infer local GB mobilities directly from sequential pairs of grain maps.

Keywords: grain growth, grain boundary mobility, diffraction-contrast tomography (DCT), machine learning.

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EUROMECH COLLOQUIUM 653
International Colloquium on Mechanics of Interfaces

August 26th-28th 2025, Metz, France

Grain boundary migration under high-cycle fatigue conditions

Brad L. Boyce[1] and Remi Dingreville[1]

Numerous nanocrystalline metals and alloys have been shown to undergo fatigue-induced grain growth. This phenomena, undocumented in textbooks on grain growth or fatigue, has been confirmed through atomistic models, in-situ TEM microscopy, in-situ synchrotron x-ray diffraction, and post-mortem cross-sectional SEM [1]. Under high-cycle fatigue conditions, this grain growth can be a rate-limiting precursor that facilitates fatigue-crack initiation. Mechanically-induced grain boundary migration and associated grain growth has been classically considered from the perspective of secondary recrystallization. In that scenario, the excess energy associated with deformation-induced dislocation substructures motivates the microstructural evolution. However, in nanocrystalline metals under nominally elastic loading conditions and with limited dislocation content, grain growth is likely not akin to recrystallization. Instead, shear coupled motion provides a more likely explanation. Such shear-coupled behavior has been rationalized at the atomic scale by coupling of stress to boundary defects, in particular disconnections [2]. Recently, this notion of disconnection-mediated boundary migration has been extended to the context of thermal cycling and postulated to also explain grain growth under mechanical cycling [3]. Anisotropic disconnection coupling gives rise to net boundary migration. Solute stabilization provides a potential pathway to control this behavior. Solute is well-known to stabilize grain boundaries against thermal evolution by a drag mechanism. In the context of mechanically-induced boundary migration, solute is known to segregate to disconnections, and can reduce the mobility of these defects [4]. Experimentally, we have been exploring this behavior a Pt-Au model alloy thin film system. Through minor additions of Au to Pt, we find substantial enhancements in fatigue resistance – far more than can be explained by solute strengthening. This stabilized alloy exhibits fatigue resistance exceeding nearly all other structural metals, withstanding cyclic strain amplitudes of 0.8% for more than 10 billion cycles – a remarkable accomplishment for a noble metal alloy system.

Keywords: fatigue; boundary migration; grain growth

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EUROMECH COLLOQUIUM 653
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Grain Growth in Nanocrystalline Metals induced by Mechanical Loading

Christian Motz[1], Jutta Luksch[1], Florentin Gaub[1], Florian Schäfer[1]

Micromechanical testing methods have made a valuable contribution to a deeper understanding of the mechanical properties and deformation mechanisms of various materials over the last two decades. In this presentation, current developments in these testing methods will be explained, with a focus on fatigue and the growth of fatigue cracks and their interaction with the microstructure.

Fatigue as well as the growth of fatigue cracks and their interaction with the microstructure play a major role in the lifespan and reliability of components. Defects in materials, such as grain and phase boundaries, but also local changes in mechanical properties due to variations in composition or grain size, can delay or accelerate crack growth. Micromechanical experiments offer the advantage of quantifying the interaction with individual "defects" in a targeted manner. For example, in-situ tests using micro-cantilevers on multilayered coatings and nanostructured metals will be presented, and the interaction between the fatigue crack tip and the microstructure will be illustrated and quantified.

We will show that cyclic plastic deformation can induce grain growth in nanocrystalline materials. Two types of experiments are performed: (i) nanoindentation fatigue and (ii) fatigue crack growth in micro bending beams. In both cases, a significant grain growth can be observed in nanocrystalline Nickel and a nanocrystalline Copper/Cobalt supersaturated solid solution alloy depending on the loading parameters. In the case of fatigue crack growth, the grain growth depends on the accumulated plastic deformation and hence, on the crack growth rate. Slow cracks show a significant grain growth in front of the crack tip, which alters the local mechanical properties. Therefore, the knowledge of the interplay between crack and grain growth is essential for understanding the reliability of nanostructured metals. Micromechanical testing methods can deliver a deeper understanding of local deformation and grain boundary migration mechanisms and establish the link to mechanical properties.

Keywords: micromechanical testing, nanoindentation, fatigue crack growth, grain boundary migration.

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EUROMECH COLLOQUIUM 653
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Dislocation-Interface Interactions in Nanoscale Eutectics

A.Ghosh [1], W.Wu[2], B. Wei[2], J. Wang[2], **A. Misra[1]**

In metallic microstructures dominated by planar interfaces such as grain or interphase boundaries, the interactions between interface-confined mobile dislocations and interactions of glide dislocations with interfaces determine the measured flow strength, strain hardening, and ductility. Dislocations can be effectively blocked at, transmitted across, deflected along, or reflected from interfaces. For grain (or interphase) boundaries involving soft metals, the efficiency of slip transmission can be predicted in terms of geometry of incoming and outgoing slip systems. However, in the case of metal-hard (intermetallic or covalent) phase microstructures, the slip system geometry, although necessary, is not sufficient to predict slip activity since the high Peierls stress of the hard phase may suppress slip transmission in favor of fracture or slip deflection/reflection from interface. Many fine-scale metal-hard phase systems show unique mechanical behavior where flow strength and ductility are simultaneously enhanced due to suppression of catastrophic localized shear bands, but there is a critical gap in knowledge of predicting the active dislocation mechanisms and relating it to the strength-strain hardening-plastic co-deformability relationship of a given soft/hard phase microstructure.

In this talk, results from recent work on developing fundamental understanding of the multitude of dislocation-dislocation and dislocation-interface interactions in *multiphase* microstructures with disparate phases will be presented. Specifically, the contribution of factors such as the thermodynamic and mechanical properties of the interphase boundary, crystallographic orientation relationships between soft and hard phases, Peierls stress of the hard phase, and morphology of the hard phase (fibrous, lamellae) in determining the relative barriers for dislocation transmission or reflection from interface will be described. Laser rapid solidified eutectic systems such as Al-Si and Al-Ge are used as model systems. The results in this investigation provide direct evidence of enabling plastic co-deformation of soft/hard disparate phase microstructure at nano-scale, through control of microstructure size, aspect ratio of hard phase, nano-twinning in the hard phase and solute segregation that may favor partial dislocation mediated plasticity.

In summary, these results suggest that microstructural *heterogeneity* at nanoscales enhances flow strength, strain hardening and *homogeneity* of plastic flow in laser processed eutectic alloys.

Keywords: dislocations, eutectics, nanomechanics, electron microscopy.

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The intricate nanomechanics of martensite interfaces, unraveled by multi-scale *in-situ* testing & advanced CP modeling

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Martensite damage in Dual-Phase steel has been extensively studied, but the exact deformation mechanisms that trigger or prevent damage initiation remain mostly unexplored. Whereas generally assumed to be hard and brittle, we revealed in '1D' nano-tensile tests that lath martensite in fully martensitic steel deforms highly anisotropically, due to sliding of the internal substructure boundaries [1]. The question is whether this interface mechanism is important in dual-phase steels and controls the damage and fracture behavior.
Therefore, various novel methodologies were developed for high-resolution and robust measurement, identification, and model validation of micromechanical deformation mechanisms. First, a new class of '2D' experiments [2] is presented that enables one-to-one quantitative comparison between microstructure-resolved mechanics in experiments – of '2D' micrometer thin specimens – and simulations – advanced crystal plasticity (CP) modeling of the full 3D phase and grain geometry of these specimens. Second, a novel nanomechanical testing and alignment framework [3], including a new nanoscale digital image correlation (DIC) patterning method [4], is introduced. Finally, **S**lip **S**ystem based **L**ocal **I**dentification of **P**lasticity (SSLIP) [5] is presented, a powerful method to measure full-field crystallographic slip system activity maps from DIC data. These slip system activity maps have been compared one-to-one to CP predictions.
These methods have been applied to study lath martensite micro-plasticity and damage in DP steel in greater detail through a combination of '1D', '2D' and '3D' experiments and advanced CP simulations [6,7]. It is shown that strong anisotropic martensite plasticity, as previously observed in fully martensitic steel, also occurs in dual-phase steels due to the specific crystallography of the martensite islands. Moreover, it was found by detailed experimental-numerical comparison that the softer martensite plasticity mechanism that occurs over the habit plane also inhibits damage initiation in martensite notches.[8]

Keywords: Martensite plasticity, Interface mechanics, SEM-DIC, Crystal Plasticity, Damage.

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EUROMECH COLLOQUIUM 653
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Grain boundary mediated deformation in a magnesium alloy at moderate temperatures and low strain rates

Berzah Yavuzyegit[1], Philip J. Withers[1], **João Quinta da Fonseca[1]**

The well-known magnesium alloy AZ31 is known to become more ductile at moderate temperatures, around 200°C. Furthermore, even when strongly textured, and therefore strongly plastically anisotropic when deformed at room temperature, it becomes essentially isotropic at these temperatures. There are two competing explanations this change in behaviour. In an influential study, Agnew and Duygulu [1] combined crystal plasticity modelling and transmission electron microscopy to make the case that it was due to enhanced <c+a> slip. However, in a later and less well -known study, Hutchinson and Barnett [2] suggested that the increase in ductility and reduction in anisotropy was instead caused by grain boundary sliding, and that <c+a> activity is not noticeably enhanced at these temperatures. Although grain boundary mediated plastic deformation is a well-accepted mechanism of deformation in nano-grained materials, it is less easy to see how it could play a major role during deformation of coarse grained materials like AZ31 sheet. Here, we present some new results of an in-situ study of a coarse grain magnesium alloy, deformed at moderate temperatures and low strain rates. Images were obtained during a long (86 hours), uninterrupted tensile test obtained using a scanning electron microscope (SEM). The sample was held at 200 °C and strained using a constant displacement rate corresponding to an average strain rate of about 1.6×10^{-6} s^{-1}, to a nominal strain of 50%. Through the use of a nano-scale gold pattern, a high resolution digital image correlation analysis of the deformation of the sample was carried out. These measurements show, for the first time, how grain boundary shearing coupled with grain boundary migration is the dominant deformation mechanism in this regime. The amount of grain boundary mobility seen, which is much higher than would expected from grain growth alone, suggests that deformation at the grain boundaries acts as a driving force for grain boundary migration. This migration helps relax the stresses associated with grain boundary shearing, and leads to alignment of the grain boundaries along the planes of maximum shear. This grain boundary mediated deformation enables the homogeneous deformation of the material, and explains the decrease and anisotropy and the increase in ductility seen at this moderate temperature and strain rates.

Keywords: grain boundary plasticity, magnesium, in-situ deformation, high-resolution digital image correlation

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EUROMECH COLLOQUIUM 653
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Electron beam induced giant ductility in amorphous Alumina (a-Al2O3) and a-Al_2O_3/Al nanolaminates

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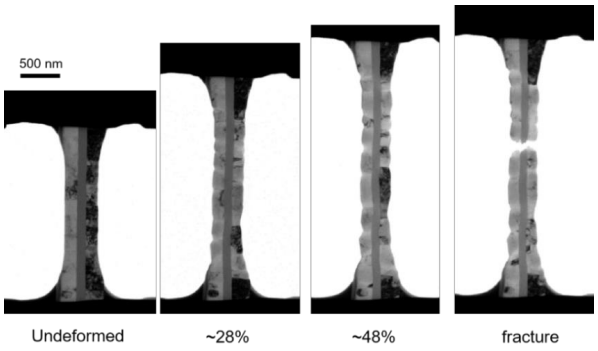
Novel technologies for, e.g., energy production, transportation, and construction demand novel materials that tolerate extremes in temperature, stress, strain rate to an extent that sometimes far exceed the limits of most advanced materials to date. Nanolaminate (NL) structures involving a high density of structural interfaces have been demonstrated as promising to meet these needs due to their unusual mechanical, electrical and magnetic properties, and radiation damage tolerance. However, up to now, only very few NL systems with nanometer-scale layers have been sufficiently studied and optimized to reach unique combinations of outstanding properties including ultra-high strength and plastic deformability, thermal stability, shock resistance, and high resistance to ion-irradiation-induced damage. In the present work, we present Al/a-Al_2O_3 NL systems involving amorphous/crystal interfaces that exhibit superior toughness, strength and ductility [1]. Recently, we used the PI-95 TEM Pico-indenter holder and the Push-to-Pull (PTP) device (Bruker.Inc) to perform quantitative in-situ tensile tests at room temperature on Al/a-Al_2O_3/Al NL model systems inside a transmission electron microscope. The results show that exposure to electron beam under tension leads to a giant ductility (more than 50%). Intriguingly, The Al layers exhibit localized necking at the majority of grain boundaries (GBs), see Figure below. This suggests GB diffusion creep is the dominant mechanism operating at low-strain rates and this feature did not manifest itself in samples deformed at higher strain rates or in the absence of electron beam irradiation. The role of the crystal/amorphous interface and the transmission of plasticity at this interface is also discussed. These findings open windows for the improvement of the ductility of hybrid crystal/amorphous NLs.



Keywords: Hybrid nanolaminate, electron beam, viscoplasticity mechanisms, in-situ nanomechanical testing

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EUROMECH COLLOQUIUM 653
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Characterization and Modeling of Interface Failure in Composites Under Complex Loading Conditions

I. Leciñana[1], L. Carreras[2], J. Renart[2], J. Zurbitu[3], B.H.A.H. Tijs[4], **A. Turon**[2]

Understanding and predicting interface failure in composite materials is essential for improving their structural reliability. This work presents an experimental and numerical investigation of delamination under multiple loading conditions, considering static and fatigue loading, evolving process zones, and the influence of loading mode history.

A benchmark test is introduced to induce non-self-similar delamination by controlling the loading conditions through block rotation. This approach enables the analysis of delamination behavior under mixed-mode loading sequences. The methodology is demonstrated using AS4D/PEKK-FC thermoplastic composites, where delamination evolution was monitored via X-ray radiography and analyzed through scanning electron microscopy (SEM) to gain insights into the fracture mechanisms.

To complement the experimental study, a cohesive zone modeling (CZM) approach is employed to predict delamination growth under complex loading scenarios. The model is validated against the benchmark test, evaluating its ability to capture process zone evolution and non-straight delamination fronts. Results show strong predictive capabilities but also highlight challenges in representing the influence of loading mode history on process zone development.

By combining advanced experimental techniques with numerical modeling, this study provides a comprehensive framework for understanding interface failure in composite materials. The findings contribute to the development of more accurate predictive models, enhancing the reliability of composite structures in real-world applications.

Keywords: Non-self-similar delamination, Failure mechanism, Loading history

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Fracture of interfaces for Printed Circuit Boards application : Experimental characterization and numerical simulations

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Driven by the increasing demands of electric mobility and power electronics, PCBs miniaturization introduces critical challenges related to reliability and durability. During operation, PCBs are subjected to thermal stresses arising from both heat dissipation in active components and environmental temperature fluctuations. These complex, multilayered structures integrate various materials with distinct thermo-mechanical properties. In particular, mismatches in their coefficients of thermal expansion (CTE) are a primary source of stress, potentially leading to delamination between insulating layers or at the copper/substrate interface.

Historically, the prevalent technique for quantifying the interfacial energy within PCBs has been the peel test, providing an estimation of the interface energy based on the IPC standard [1]. However, during peeling, copper tends to experience large plasticity. Consequently, the analysis of peel tests with plasticity developement in the film has been extensively explored in the literature [2]. More recently, in [3] and [4], focusing on the elastic-plastic response of copper (Voce and/or Kinematic hardening), the peel test has been analysed to identify the cohesive behavior of the substrate/copper interface. Nevertheless, it has been observed that this approach is challenging when seeking a precise evaluation of the mechanical response of the interface.

To tackle this challenge, Double Cantilever Beam (DCB) and End Notched Flexure (ENF) tests [5], originally designed for thick composites, have been adapted to the PCB domain, where layers are is significantly thin, with copper traces thickness ranging from 17 to 70 µm. Prior to experimentation, the test configurations were validated through finite element (FE) simulations, it was demonstrated that the plastic dissipation in the DCB and ENF setups is drastically reduced when compared to the one observed in peel tests. Beyond estimating the critical strain energy release rates in Mode I and Mode II (GIc and GIIc) and the corresponding critical stress, these combined experimental and numerical approaches establish a robust framework for evaluating the limitations and the applicability of these methods to PCB interfaces.

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Key Words: *Finite element method, Traction-Separation Law, Double Cantilever Beam, End Notched Flexure, Printed Circuit Board (PCB)*

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EUROMECH COLLOQUIUM 653
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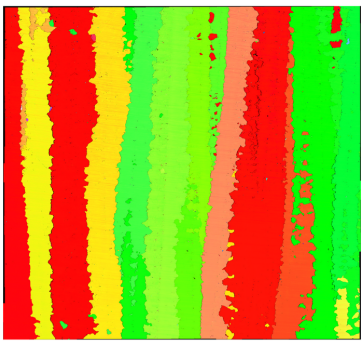
Full field modelling of viscoplasticity and intergranular damage in directionally solidified nickel-base superalloys

Ayoub El-Habyb[1], Jean-Michel Scherer[1], Kais Ammar[1], Florent Coudon[2], Louis Augustins[2], **Samuel Forest**[1]

Keywords: Crystal plasticity, grain boundary damage, unilateral damage, DS superalloys

Directionally solidified nickel-base superalloys used for turbine blade applications in jet engines or gas turbines have a complex microstructure consisting of columnar grains separated by long and corrugated grain boundaries, shown below. Under creep loading conditions, especially along the transverse direction, the grain boundaries are subjected to oxidation and subsequent intergranular damage [1]. A constitutive model is developed that combines single crystal viscoplasticity inside the grains and a specific damage behaviour law that includes normal and tangential damage in a diffuse region around grain boundaries parametrized by a phase field variable [2,3]. Material parameters are calibrated at two temperatures from tensile and creep tests along the solidification and from transverse creep test results. Specific unilateral damage conditions are implemented to account for crack closure effects that inevitably occur due to the complex GB geometry.



Microstructure and crystallographic texture of a directionally solidified nickel-based superalloy

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The Role of Longitudinal Twin Boundaries on the Distribution of Failure Strains of Metallic Nanowires

Rohith Polisetty[1,2], **Dan Mordehai[1]**

The mechanical behavior of polycrystalline metallic nanowires is strongly influenced by the interaction between dislocaitons and grain boundaries, which govern deformation mechanisms and failure processes. In this study, we employ molecular dynamics (MD) simulations to investigate the role of longitudinal twin boundaries (LTBs) in the plasticity and ductility of bicrystalline gold (Au) nanowires and penta-twinned silver (Ag) nanowires. By systematically varying the nanowires' cross-sectional shape, aspect ratio, and grain dimenstion, we analyze how these structural parameters affect strain to failure by simulating several realizations for each case. For bicrystalline Au nanowires, we find that deformation initiates through the nucleation of Shockley partial dislocations from nanowire edges, followed by their interaction with the LTB [1]. This interaction leads to two competing mechanisms: detwinning of the LTB, which results in crystal reorientation, and dislocation slip. The relative dominance of these mechanisms varies stochastically, leading to a distribution in detwinned volume fractions and failure strains. Notably, the extent of detwinning correlates linearly with strain to failure, showing that nanowires with more symmetric grain configurations exhibit lower ductility. In contrast, penta-twinned Ag nanowires deform through stacking fault formation, which dictates their failure behavior. While yielding occurs via the nucleation of Shockley partial dislocations, variations in their interactions lead to different microstructural evolutions, sometimes resulting in void formation at the nanowire center. This process contributes to larger failure strains, as confirmed by a modified Weibull statistical analysis of the failure strain distribution. By comparing these two systems, we provide insight into how different twin structures mediate plasticity and failure at the nanoscale. Our findings highlight the critical role of the initial mirostructure in dictating mechanical performance and offer guidelines for designing nanostructured materials with enhanced ductility and tailored mechanical properties.

Keywords: Bicrystalline Au nanowires, penta-twinned Ag nanowires, molecular dynamics simulations, failure strain.

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Effect of strain rate and grain size on the oxidation-assisted intergranular cracking of the Alloy 718 at 650 °C

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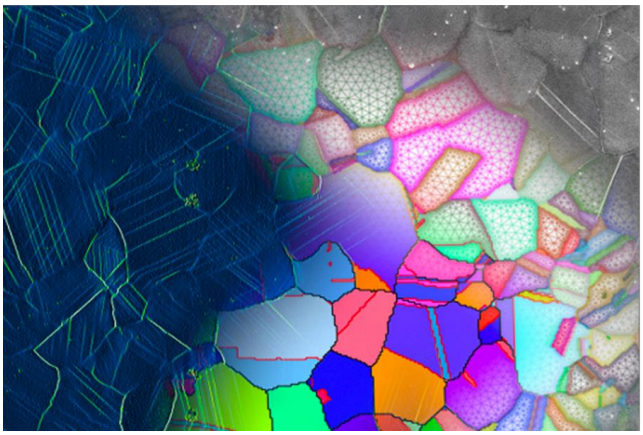
Keywords: Ni-based superalloy, high resolution digital image correlation, slip localization, grain boundary sliding.

The Ni-based superalloy Alloy 718 (Inconel 718) is an excellent alloy candidate for structural components operating at intermediate temperatures. In the past decades, its mechanical behavior and damage behavior has been intensively investigated at high temperature to establish a relationship between its strain-rate sensitivity and its oxidation-assisted intergranular cracking (OAIC). The present study focuses on the effect of the temperature [1], the strain rate [2] and the grain size [3] effects on strain localization partitioning at grain boundaries (GBs), twin boundaries (TBs) and intergranular from room temperature up to 650 °C, in the Portevin-Le-Chatelier (PLC) and non-PLC domains. HR-DIC analysis and out-of-plane measurements using laser scanning confocal microscopy were performed to quantify plasticity distribution and preferential cracking site at the microstructure scale depending on the strain rate. A particular attention was paid on the slip band/grain boundary interaction to better document damage development at grain boundaries and transition from strain localization to early damage. Changes in strain localization with the grain size and strain rate demonstrated the concomitant action of strain localization and environmental degradation on the OAIC.



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EUROMECH COLLOQUIUM 653
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Low-stress deformation and early fracture at basal twist grain boundaries in titanium alloys

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Recent investigations of fatigue failures highlighted crack nucleation at basal twist grain boundaries (BTGBs) in near-α and α+β titanium alloys [1,2]. Preliminary slip activity is generally acknowledged as a critical step due to irreversible deformation eventually leading to fatigue crack formation. A prior study highlighted that early slip activity can proceed at these specific microstructure configurations, however the understanding of underlying mechanisms and critical features remains insufficient [3]. The presently reported study addresses this gap of knowledge.
Large area mappings were first carried out using electron back-scattered diffraction to collect statistical information about the BTGB population in an engineering Ti-6Al-4V alloy with an equiaxed microstructure. Quantitative characterization of deformation at a selection of BTGBs was then performed in-situ using in-SEM tensile tests combined with high resolution digital image correlation. This methodology enabled a comparison with other slip events, and the analysis of interactions with the surrounding microstructure. In addition, new insights into the fracture behavior were obtained increasing the macroscopic strain in-situ until the formation of cracks. Collected data was examined to identify key features associated with the most critical configurations. Complementary atomistic simulations were finally performed to provide further information about the grain boundary structure, and simulate the response of BTGBs under shear loading. Underlying mechanisms and the effects of microstructural characteristics, such as the tilt and twist components, were unravelled in light of these results.

Keywords: Deformation, fracture, grain boundary, titanium, fatigue

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Deformation Twinning in Metals with Hexagonal Close-Packed Crystal Symmetry: network formation and stability

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Keywords: Deformation twinning, twin networks, plasticity, hexagonal close-packed

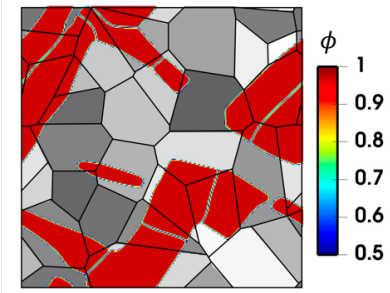

Figure 1. (a) Snapshot showing the deformation twin microstructure predicted by the multi-phase field-crystal plasticity framework at 190 ps.

Deformation twins play a key role in accommodating strain during plastic deformation in hexagonal close-packed (hcp) metals and their alloys. The typical deformed microstructure in hcp polycrystals corresponds to a relatively complex and interconnected 3D twin network. The role of the nature/fingerprint of the twin network on plastic flow and failure remains unclear. To unravel how twin networks form, we study the full 3D character of deformation twins and their associated networks, using a combination of experiments, models, and theory.

Using a 3D-electron backscatter diffraction (3D-EBSD) characterization approach combined with a graph theory-based code to reconstruct and analyze twin networks in 3D and in 2D, we reconstruct complex twin networks in pure Ti and demonstrate that: (i) 2D characterization of twin networks do not provide a representative view of the connectivity of twin networks/number of twin transmission events/ number of co-nucleation events and, (ii) twin networks in deformed Ti are particularly dense and connected largely in consequence to twin transmission events (see Ref 1 and 2). Using convolution neural network, we further analyze the key features of the microstructure best correlating with successful twin transmission and infer that that local stresses and maximization of dissipation potential dominate the twin transmission process rather than geometry (e.g. grain boundary normal). Using a novel crystal plasticity phase field formalism alongside theoretical derivation we further study the impact of local internal stresses, such as those emanating from dislocations on the twin network formation. The simulations rationalize the observed complex twin network morphologies thereby illustrating the critical role of co-deformation (i.e. slip and twinning) on twinning.

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Detwinning and the twin/matrix interface strength in FCC materials

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Three different detwinning systems may be activated in face-centered cubic metallic materials and the experimental results have revealed different critical resolved shear stresses of these systems as well as other physical differences [1,2]. Temperature dependence of the detwinning stress of face-centered cubic deformation twins were evaluated studying the effect of elevated temperatures on plastic deformation properties of multilayered twin/matrix structure of the Cu-8at.%Al alloy [3]. The critical resolved shear stress of detwinning was found to increase with temperature when plastic yielding of the twin/matrix structure occurred by the reverse detwinning mode (π mode). However, when an alternative quasi-reverse mode of detwinning (π/3 mode) was involved, a decrease of the critical resolved shear stress with an increase of temperature was observed, instead. Thus, the twin/matrix structure behaved in two opposite ways, showing anneal hardening in the case of π mode and anneal softening in the case of π/3 mode upon temperature increase. As concluded, the dual effect of temperature on the detwinning stress resulted from irreversible reduction of internal stresses pre-existing within the deformation twins. The complete reduction of the internal stresses at about 530◦C led to the equivalence of the critical stresses of different detwinning modes and to a large decrease of the yield stress anisotropy of the twin/matrix structure. It is postulated that temperature induced annihilation of the internal stresses resulted from constriction of extended cube dislocations pre-existing within deformation twins. The temperature limit of about 540 ◦C, beyond, which the twin/matrix structure became unstable due to recrystallization, was also established. Moreover, transfer of plastic shear throughout the twin/matrix structure was found to be predominantly controlled by internal dislocation substructure of deformation twins, not by the twin/matrix interfaces.

Keywords: twinning, twin-matrix interphase, dislocations, tensile tests.

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EUROMECH COLLOQUIUM 653
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Elastic strain measurement at particle-matrix interfaces and at dislocations pile-ups by TEM

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Many phenomena develop elastic strains at the nanoscale, for example dislocation pile-ups and coherent precipitation. Yet, because of their small scale, these elastic strains are rarely measured. In this work, we developed a method of elastic strain mapping in the TEM and applied it to the study of several cases. Elastic strains and micro-rotation are calculated from the shifts of the diffraction spots position between the nano-diffraction patterns acquired in the field of view and a reference pattern taken from an unconstrained region of the crystal. The spatial resolution is ~1nm and the fields of view can reach several microns.

In the first case, the elastic strains are mapped around a coherent Al_3Sc precipitate in an aluminium alloy. The measurements agree very well with the theoretical predictions of the Mott-Nabarro model. In the second case, the elastic strains and micro-rotation developed at dislocations walls and pile-ups are evidenced in a Cr_2AlC crystal. The observations are in strong agreement with the theoretical models for strains developing at dislocation pile-ups. The differences and complementarity of this technique with other techniques of elastic strain measurement (HR-EBSD, µLaue) are highlighted, and finally the potential of the technique for the study of strains at interfaces is discussed.

Keywords: Elastic strains, TEM, coherent particles, dislocations

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The role of matrix-twin interfaces in the void growth in HCP crystals

Saketh Virupakshi[1], **Katarzyna Kowalczyk-Gajewska** [2]

The growth and coalescence of voids in HCP magnesium single crystals deforming through slip and twinning are examined using CPFEM, by employing a unit cell methodology. A 2D plane strain geometry with a cylindrical void and a 3D one with a spherical void are considered. A rate-dependent crystal plasticity model is used, accounting for slip and twinning interactions, and employing predominant twin volume consistent reorientation scheme [1]. For a better understanding of the impact of stress state on void growth, simulations were conducted using constant stress ratio controlled boundary conditions imposed through a special spring element as in [2]. The crystal plasticity model parameters and deformation modes representing the Mg alloy AZ31B were used in the calculations. Different crystal orientations with respect to principal loading directions are selected leading to the various deformation scenarios. In particular, for the cases when twinning is active we observe microstructure evolution related to the appearance of domains of new twin-related orientation. Appearing matrix-twin interfaces have an impact on the void growth, namely the early phase of void formation is greatly hindered due to twinning activity and influences the mode of material failure (either by shear localization or void coalescence), Fig. 1. Next, due to the activity of multiple slip systems in twinned region after reorientation, the textural hardening of the crystal matrix is seen, the void growth rate is increased.
Acknowledgments: The research is partially supported by the project No. 2021/41/B/ST8/03345 of the National Science Centre, Poland

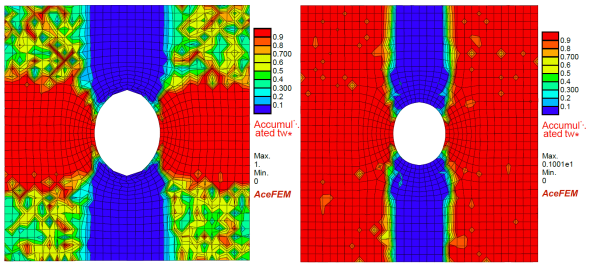

Fig.1 Accumulated twin: 2D unit cell with stress ratio: 0.8 (left) and 0.4 (right) at strain 0.05 in principal loading direction.

Keywords: void growth, twinning, finite element, crystal plasticity.

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EUROMECH COLLOQUIUM 653
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Density Functional Theory of Interphases

Sabine Enders[1]

In chemical engineering, the material has to be transported via the interphase, where the interface properties are dependent on the temperature, the pressure and the composition of the mixture. The temperature, pressure as well as composition of the mixture can be modelled using an equation of state (EOS) in combination with standard thermodynamics. Usually, the EOS describe the coexisting fluid phases, where the spatial resolution of the physical properties is not required. In contrast, the physical properties within the interface depended on the special position in the interface. This conflict can be solved by the classical density functional theory (DFT) [1]. The combination of the EOS with the DGT results in an expression of the Helmholtz energy $F\left(T,V,x_i\left(z\right)\right)$, where T is the temperature, V is the volume, and $x_i\left(z\right)$ is the mole fraction of component, i, and z is the perpendicular position in the interface. The minimization of $F\left(T,V,x_i\left(z\right)\right)$ yields the interfacial properties, like the interfacial tension and the concentration profiles, $x_i\left(z\right)$. The latter information can be used to figure out the components, which will be enriched in the interface.
This concept was applied to different interphases, for instance, vapor-liquid interphases [2], and liquid-liquid interphases [3], as well as to the adsorption of fluids on solid surfaces [4]. The concept can also be used if chemical reactions take place and consequently, the interfacial properties depend additionally on time [5].

This contribution will focus on the modelling of adsorption isotherms for two examples. The first example is the adsorption of small gases on active carbons or zeolites. The second example is the separation of isomers. It turns out, that the modelling of the solid surface is the bottleneck for this approach. Therefore, possible cooperation with the mechanic community will be discussed.

Keywords: Density Functional Theory, Equation of State, Adsorption

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EUROMECH COLLOQUIUM 653
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Towards a better understanding of hydrogen implication on intergranular fracture in nickel-based alloys

A. Oudriss[1], J. Bouhattate[2], **X. Feaugas[3]**

Among the significant effects of the environment on mechanical properties, hydrogen is often cited as a determining vector in the weakening factors. In many situations in nickel-based alloys, hydrogen leads to intergranular fracture, the mechanisms of which remain to be clarified. In accordance with this challenge, we examined the metallurgical factors that influence the ingress, diffusion, and trapping of hydrogen within a polycrystalline aggregate. We show that the diffusion of hydrogen is anisotropic at bulk, as in subsurface within the grain [1,2]. On the other hand, grain boundaries appear as a short circuit of diffusion or trapping sites depending on their nature (misorientation, energy …) [3,4]. To arrive at a classification, the solute/defect interaction energy is used to discuss the trapping of hydrogen on vacancies, dislocations, precipitates, and grain boundaries. Secondly, we question the involvement of hydrogen in plasticity mechanisms [5-10]. By challenging the influence of hydrogen on elasticity and the short- and long-range interactions between dislocations, we demonstrate the antagonistic hardening/softening effects.
At the end of these two approaches, we question intergranular fracture in relation to the nature and distribution of grain boundaries but also the internal length scales developed in plasticity in the presence of hydrogen [10].

Keywords: Hydrogen, vacancies, dislocation organisations, grain boundary, diffusion, plasticity, intergranular fracture.

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Multiscale modelling of electro-chemo-mechanical interactions in particle composites with material interfaces

David Rollin[1], Fredrik Larsson[2], Kenneth Runesson[2], **Ralf Jänicke[1]**

Computational modeling of batteries is crucial for advancing energy storage by enabling simulation and optimization of materials and processes. Batteries involve complex electrochemical, transport, and mechanical interactions across multiple scales. Key challenges include non-linear diffusion, phase interactions, and mechanical degradation. Electrochemical processes and mechanical properties are tightly coupled, as mechanical stress affects ion transport and interfacial stability, while electrochemical reactions induce deformation [1,2]. Particle-matrix composites in electrodes add complexity due to reaction kinetics and mechanical effects at material interfaces. Accurate homogenization techniques bridge microstructural behavior with macroscopic performance, reducing reliance on costly experiments and Direct Numerical s Simulations.

This study examines computational homogenization of particle-matrix composites with material interfaces, using linear transient diffusion driven by a chemical potential as a model problem. To balance computational efficiency and accuracy, we assume micro-stationarity, allowing direct upscaling without expensive time-dependent microscale simulations. As a baseline, first-order homogenization with a single macroscale chemical potential is considered but fails to capture micro-transient effects.

To overcome this, we propose an alternative approach with dual macroscale potentials, one per material phase, while maintaining stationary subscale computations [3]. Two prolongation strategies are explored: constant-linear and linear-linear. For the latter, we assess different methods for defining macroscale variables in the Representative Volume Element (RVE) problem: (i) averaging the 0th and 1st gradients of the chemical potential and (ii) averaging the 0th and 1st moments of the potential. A detailed numerical study evaluates the performance of these methods against a reference Direct Numerical Simulation (DNS) solution.

Keywords: Computational homogenization, multiphysical modelling, resistive interfaces.

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From voxels to interfaces: adapting FFT-based methods for geometric accuracy

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Crystal plasticity (CP) models are increasingly used in scale-bridging applications to obtain microstructure-sensitive mechanical response of polycrystalline materials. These models require a proper consideration of the single crystal deformation mechanisms, a representative description of the microstructure, and an appropriate scheme to connect the microstates with the macroscopic response. FFT-based methods originally proposed for composites [1] and extended to polycrystals [2] are attractive due their higher efficiency compared with CP-Finite Elements, and their direct use of voxelized microstructural images. In this talk, we will report recent progress on FFT-based polycrystal plasticity, with emphasis in novel implementations, including strain-gradient plasticity, achieving geometric accuracy working with voxelized images, non-periodic extensions, and dynamic effects. We will show applications of these methods to study the role of interfaces in plasticity, interactions between interfaces and waves in elastically heterogeneous materials, multiscale coupling with Lagrangian hydrocodes, and integration with 3-D characterization methods.

Keywords: Crystal plasticity, polycrystals, FFT-based methods

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Grain boundary constitutive equations implemented in a strain gradient FFT-based formulation

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Dislocation interactions with interfaces are governing the behaviour of certain lamellar composites (e.g. nanometallic laminates) and fine-grained materials, and phenomena such as slip localization and transmission in polycrystals. Strain gradient crystal plasticity micromechanical models account for the effects of geometrically necessary dislocations and can simulate large volumes of material. However, effects of interfaces on dislocation flow are usually oversimplified. Most of the published models adopt either free flow (micro-free), or zero flow (micro-hard) Burgers vector conditions at an interface [1]. Gurtin and Needleman proposed a general method for treating a grain boundary (or an interface) in the context of strain gradient plasticity [1]. They assumed that the power at the grain boundary is spent only on Burgers vector accumulation within the boundary, and derived the corresponding grain boundary constitutive relations. Due to the complexity of the resulting system of equations, the proposed grain boundary expressions were not numerically implemented in strain gradient models and thus were not compared with experiments. In this work, we propose two novel expressions for power spent at a grain boundary and derive the corresponding grain boundary constitutive equations by following the methodology originally developed by Gurtin and Needleman [1]. We implement the grain boundary constitutive equations proposed by Gurtin and Needleman and the two novel expressions in a strain gradient FFT-based micromechanical model first developed by [2] and study the resulting Burgers vector flow and accumulation at grain boundaries for the case of Cu-Nb nano-metallic laminate and a fine-grained polycrystal [3]. It is found that the constitutive equations proposed by Gurtin and Needleman result in a significant flow of Burgers vector from one side of the boundary to the other regardless of the adopted boundary resistance, leading to weak dislocation pile-ups at grain boundaries, in contradiction with experimentally observed behaviour for studied materials. The two new grain boundary equations proposed here allow full suppression of dislocation flow at the grain boundary with the increase of the boundary resistance, and thus larger dislocation pile-ups in better agreement with experiments.

Keywords: strain gradient plasticity, FFT, dislocations

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EUROMECH COLLOQUIUM 653
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August 26th-28th 2025, Metz, France

A size-dependent homogenization scheme for gradient plasticity in periodic laminates

Claudius Klein[1], Thomas Böhlke[2]

The quantitative prediction of macroscopic mechanical properties of materials requires the consideration of the material microstructure. This talk focuses on metallic material systems with lamellar microstructures, such as NiAl-Cr(Mo) or binary Fe-Al [1,2]. These consist of individual domains in which the materials constituents are arranged in fine layers (thickness in the micrometer range) with a distinct layer normal direction. The layer interfaces act as obstacles for dislocations, leading to dislocation pileups which influence the macroscopic stress response via a size-dependent evolution of the defect structure and the corresponding back stress in the laminate on the micro scale. The back stress leads to an increase of the macroscopic yield stress through size-dependent kinematic hardening, which is observable upon load reversal.

In order to model the material system, we make use of a two-scale homogenization approach. For this, we describe the microstructure of one domain as a periodic rank-1 laminate, which allows for efficient mathematical description of the mechanical behavior of one domain. Exact localization relations are used to explicitly resolve the local stress and strain fields. Within the framework of gradient crystal plasticity [3,4], the yield conditions take the form of a system of coupled Fredholm integro-differential equations for the plastic slip, which is solved semi-analytically under consideration of the loading-unloading conditions. This size-dependent modeling approach allows for a physically motivated description of the Hall-Petch and the Bauschinger effect, taking both the lamella widths as well as the lattice orientation of the different constituents into account. The capabilities of this method are demonstrated by means of multiple examples where the influence of different microstructure parameters are discussed.

Keywords: micro mechanics, lamellar morphology, gradient plasticity, size effect

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EUROMECH COLLOQUIUM 653
International Colloquium on Mechanics of Interfaces

August 26th-28th 2025, Metz, France

Mean Field Modeling Including Interface Energies

Thomas Böhlke[1], Frederik Hille[2], Sabine Enders[3]

Homogenization methods in mechanics and thermomechanics allow the calculation of effective mechanical properties of solids [1, 2] and fluids [3] based on information about the material's microstructure and the constitutive properties at the micro level. Additionally, in many cases, the fluctuations of the mechanical fields at the micro level can also be determined [4]. Typical homogenization methods include mean-field approaches and FEM- or FFT-based full-field methods. Examples of homogenized thermomechanical properties are elastic stiffness, thermal stresses or strains, thermal conductivity coefficients, heat capacities, yield stresses, or creep strains. In most cases, only the bulk properties are considered in the homogenization methods, so interfacial energies at the micro level do not enter into the predictions of the effective properties.

In the presentation, we address the possibility of considering interfacial energy in thermomechanical homogenization approaches with focus on mean-field approaches. Selected examples of interfaces in fluids and solids are discussed, addressing both equilibrium and non-equilibrium solutions. It is shown how interfacial energy can influence the effective properties, especially in systems with a high number or density of interfaces.

Another important aspect is the consideration of interfacial energy in the modeling of phase transitions and the associated mechanical and thermal properties. Both experimental and theoretical approaches can be used to quantify the interactions at the interfaces and integrate them into the homogenization models. This enables more precise predictions of material properties and contributes to the development of new materials with tailored properties.

Keywords: Micromechanics, Homogenization, Interface Energy, Phase Transition

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Size-dependent patterns of propagating instabilities in shape memory alloy tubes

Mohsen Rezaee-Hajidehi[1], Elham Sarvari[2], Aslan Ahadi[2], Stanisław Stupkiewicz[1]

It is commonly observed in the experiments that stress-induced martensitic transformation in polycrystalline shape memory alloys (SMAs), particularly in textured NiTi, initiates through deformation instability and progresses via the propagation of diffuse patterned interfaces, forming a macroscopic transformation front. This process is accompanied by a stress drop and a stress plateau in the mechanical response of the SMA specimen. The phenomenon of instability in SMAs is now well understood to stem from a non-monotonic (involving a softening regime) intrinsic material response, a particular feature that can be attributed to the formation and annihilation of transformation interfaces at the single-grain level [1].
The spatiotemporal heterogeneity arising from a localized transformation evolution significantly influences the mechanical characteristics of the material and in particular its fatigue behavior [2]. This raises critical questions and poses serious challenges in the implementation of SMA components in practical applications. Of special interest are NiTi tube-based devices that have gained prominence in advanced applications due to the performance advantages they offer. Notable examples include their use in cardio-vascular stents, elasto-caloric cooling devices and neurosurgical procedures. In these applications, NiTi tubes of various dimensions experience distinct deformation modes, which makes it essential to characterize their size-dependent deformation/transformation behavior in order to optimize the performance and reliability. Motivated by this, the present study aims to elucidate the impact of tube diameter and wall-thickness on the pattern of propagating instabilities in NiTi tubes under quasi-static uniaxial tension and pure bending. The application of multi-magnification and high-resolution stereo digital image correlation (DIC) technique has facilitated a precise capture of localized strain fields in micro-scale tubes [3]. The results of our recent DIC-based experiments have revealed the emergence of a diverse range of transformation patterns in tubes with different sizes, from a front possessing multiple fingers (bands) in large and slim tubes to a fingerless flat front in small and thick tubes. We employ a gradient-enhanced model of superelasticity to validate our experimental observations and to interpret the size-dependent transformation front patterning based on the competition between the interfacial energy of the front and the elastic strain energy stored in the tube.

Keywords: Shape memory alloys; Superelasticity; Transformation pattern; Finite-element analysis

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Identifying the role of interfaces on mechanical properties of polycrystalline alloy by encoding microstructure and plasticity

M. Calvat[1], C.Beam[2], D.Anjaria, **J.C. Stinville**

We encode metal plasticity from high-resolution digital image correlation captured during elementary loading conditions to predict monotonic and cyclic macroscopic properties in metallic materials. Simultaneously, microstructure information is captured from the encoding point diffraction data. To preserve spatial heterogeneity information, latent space features of both plasticity and microstructure are mapped across large fields of view while maintaining their original spatial relationships from the experimental measurements. This results in latent space feature maps that effectively capture the complexity and heterogeneity of metal plasticity and microstructure in a low-dimensional representation. These maps are then leveraged to train a convolutional neural network-based model for predicting macroscopic properties and analyzing the role of interfaces. The approach is demonstrated on a large dataset of face-centered cubic metals. Finally, we assess the role of interfaces in mechanical properties through latent space feature analysis.

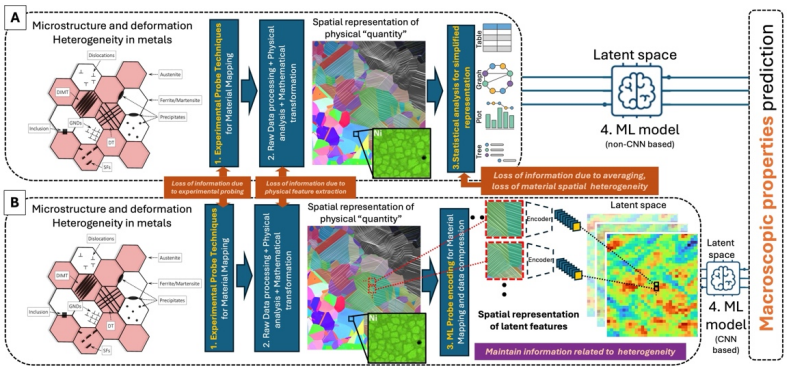

Figure 1: In the conventional approach, microstructure and deformation fields are measured using experimental probing techniques. Subsequently, discrete metrics or simplified representations are extracted to relate these measurements to macroscopic properties. Significant information loss occurs due to data averaging, notably the loss of spatial heterogeneity, a critical factor influencing macroscopic properties. Adapted from 9, 17, 18. (B) The proposed approach differs primarily in the final step, where encoders compress the data into a latent space. This compressed representation is combined with latent space feature mapping to preserve spatial heterogeneity while remaining sufficiently reduced for use in data-based models

Keywords: Variational autoencoder, plastic localization, mechanical properties, materials informatics
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Correlative Diffraction Microscopy Imaging experiments to investigate crystal plasticity

Henry Proudhon[1], Wolfgang Ludwig[2], Clément Ribart[1], Daria Mesbah[1], Maryse Gille[1]

Key mechanical properties such as tensile strength or fatigue limit of metallic structural materials are to a great extent governed by the three dimensional arrangement of the material microstructure. Both synchrotron and laboratory X-ray based characterization methods now allows for non destructive analysis and in situ multi-modal, correlative measurements in microstructures containing thousands of grains. This has the potential to revolutionize material characterization, deformation and fracture mechanisms investigations, as well as constitutive behaviour identification at the grain scale.

This presentation will showcase results from several studies which bring new insight on crystal plasticity of structural metallic materials. Different characterization modalities can now be combined on the same sample such as EBSD, HR-DIC, (lab or synchrotron based) DCT and Topotomography at different stage of tensile deformation, sometimes in situ, sometimes ex situ. Formations of deformation structure at different scales such as sub grains, slip bands and shear bands can now be accessed non destructively in the bulk [1, 2]. In all cases, measuring the same grains with different modalities brings new insight on crystal plasticity mechanisms and their interaction with the grain boundary network.

In addition, having access to the whole 3D microstructure allows to create digital twin representation of the material piece to test its mechanical behaviour *in silico* using either crystal plasticity FFT or FEM methods. This enables to access non measurable quantities, validate grain scale material models and could also represent new avenues for rapid material model identification methods.

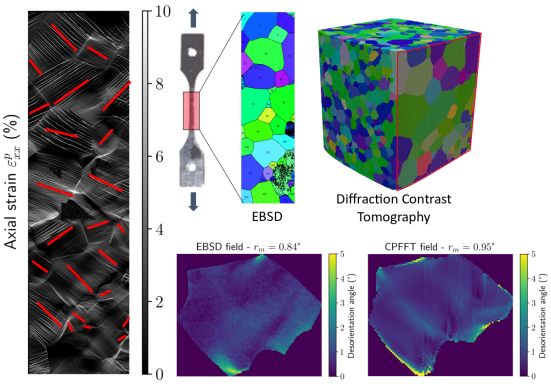

Fig. 1: Exemple of multimodal study of deformation mechanisms in pure titanium.

Keywords: X-ray tomography, in situ mechanical testing, crystal plasticity, deformation and fracture.

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A general imperfect interface model for strain-gradient elasticity

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Interfaces are present almost everywhere in mechanics, physics and engineering. The present work aims to extend to strain-gradient elasticity an efficient and fruitful approach of constructing physically meaningful imperfect interface models[1]. The motivation for this work is twofold. Indeed, within the framework of strain-gradient elasticity, the interfacial continuity and discontinuity relations have not yet completely been provided even for the perfect interface in the relevant literature, and a general model is still lacking for imperfect interfaces.

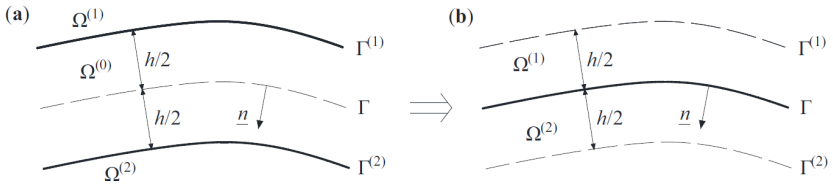

Fig 1. (a) Three-phase configuration in which a thin interphase occupying $\Omega^{(0)}$ is perfectly bonded to phases 1 and 2 occupying $\Omega^{(1)}$ and $\Omega^{(2)}$; (b) Two-phase configuration in which the interphase $\Omega^{(0)}$ is replaced by an imperfect interface Γ, and phases 1 and 2 are extended up to the imperfect interface Γ.

In the first part of our work, the interfacial continuity and discontinuity relations are completely and explicitly given for the perfect interface of strain-gradient elasticity. These relations are formulated mathematically in a compact way by introducing a set of orthogonal projection operators. These operators are novel and play an important role in strain-gradient elasticity.

In the second part of our work, to derive a general physics-based imperfect interface model, two configurations are considered (Fig. 1): (a) a three-phase configuration where a very thin interphase of constant thickness occupying the domain $\Omega^{(0)}$ is perfectly bonded to phases 1 and 2 occupying the domains $\Omega^{(1)}$ and $\Omega^{(2)}$; (b) a two-phase configuration where the interphase is replaced by an imperfect interface geometrically located at the middle surface Γ of the interphase and phases 1 and 2 are extended to the middle surface Γ. The general imperfect interface model is characterized by: (i) the displacement vector jump relation; (ii) the traction vector jump relation; (iii) the normal displacement gradient jump relation; (iv) the double traction vector jump relation. These relations are established by using asymptotic analysis while accounting for the interfacial continuity and discontinuity relations obtained in the first part for the perfect interface. When these relations are satisfied, the configurations (a) and (b) are equivalent to within an error of order $0(h^2)$. The orthogonal projection operators introduced turn out to play an essential role in dealing with interface problems in strain-gradient elasticity.

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