

DISLOCATIONS 2008

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Book of Abstracts

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A new model for dynamic recovery in Stage III deformation of FCC metals

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Since the early researches on the strain hardening of FCC metals in the 50s by Seeger and others who followed, it has been generally accepted that dynamic recovery in Stage III deformation of FCC metals is controlled by massive cross slip of screw dislocations, circumventing linear Lomer-Cottrell (LC) dislocation barriers and results in decreasing strain hardening rates. Apart from fragmentation of slip bands and the dependence of τ_{III} on stacking fault energy, which can both be explained differently, this proposition is quite inconsistent with the cellular dislocation microstructure that develops in Stage III hardening, and can not provide a rational explanation of its self similar reduction in scale with increasing plastic resistance.

In a proposed new mechanism dynamic recovery results from the systematic removal of LC locks in cell walls under the repeated impingement of dislocation fluxes that, in turn, trigger associated collapse events in much of the pinned redundant cell wall dislocation microstructure. This then provides the required kinematic degrees of freedom for displacement of cell walls and permits the flow-noise-induced cell refinement process of Haehner and Zeiser, to develop unhindered. The model correctly predicts the onset of dynamic recovery at τ_{III} , its dependence on temperature and stacking fault energy, as well as the temperature and stress dependence of the decreasing strain hardening rate of Stage III, referred to as the Voce Law.

Dislocation climb plasticity: modelling and comparison with the high-temperature mechanical properties of quasicrystalline AlPdMn, and superalloys

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We propose a model which fully accounts for several unexplained aspects of the mechanical properties of icosahedral AlPdMn, published in the literature. This model is based on *post mortem* and *in situ* TEM observations of two dislocation families moving by pure climb and exchanging vacancies. It provides the first direct evidence of the chemical (or osmotic) force induced by an out-of-equilibrium vacancy concentration. It relies on the following properties which can be considered as the signature of pure climb plasticity:

- a high strain-hardening at yield, due to a strong decrease of the concentration of vacancies consumed by climbing dislocations,
- a steady-state flow stress twice higher than the elastic limit, which is accounted for by the equilibrium value of the chemical stress,
- two-stages relaxation curves defining strain-rate sensitivities in a ratio of 2, which are a direct consequence of the complex relaxation of the chemical stress.

The true stress-dependence of the dislocation climb velocity, which has been determined accordingly, is different from the linear dependence given by classical models valid at low stress. It is however in a fair agreement with the model of Hirth and Lothe, which describes the nucleation of jog pairs on straight dislocation segments observed in TEM. The best fit is obtained for a jog height of about 1nm, i.e. of the order of the average distance between cluster rows.

These conclusions may be transposed to crystals deformed under specific conditions favouring pure climb deformation. The high-temperature creep of superalloys, in which climbing dislocations also exchange vacancies, will be treated as an example.

Introducing Dislocation Climb by Bulk Diffusion in Discrete Dislocation Dynamics Simulations

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One of the powerful computational tools to study dislocation microstructure and plasticity at the mesoscopic scale is Dislocation Dynamics simulations, in which dislocations are treated as elastic entities. In this talk, we present a method to incorporate dislocation climb by bulk diffusion in Dislocation Dynamics simulations, by coupling this simulation technique with the diffusion theory of vacancies. We adapt the method to a 3-dimensional Discrete Dislocation Dynamics (DDD) simulation, in which each dislocation is represented by pure edge and screw dislocation segments. We firstly discuss the case in which the interaction between the flux fields of climbing segments is omitted. The calculation is demonstrated by simulating the activation of a Bardeen-Herring climb source upon the application of an external stress or under vacancy supersaturation, as well as isolated dislocation prismatic loops shrinkage and expansion. The model is then extended to allow climb in bulk materials, where dislocations are sources of vacancies, by considering simple interaction between the segments' flux fields. Subsequently, the model is shown to reproduce the coarsening of dislocation loops in annealed bulk. We observe in our simulations that large dislocation loops expand on the expense of smaller ones. Medium size loops are found to translate from expansion to shrinkage, as the vacancy supersaturation is relieved along the calculation. The processes observed in our simulations agree with experimental observations in fcc metals.

Mechanistic Insights for Modeling Dislocation Climb

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The interaction between dislocation climb and glide is a central issue in understanding creep. While there are atomistic methods to treat glide, the study of climb is still a challenge. The long time scale nature of dislocation climb mandates that modeling such phenomenon requires coarse graining the atomistic details of one or more vacancies binding to dislocation core. We use an empirical interatomic potential for BCC Fe¹ to obtain atomistic details of vacancy diffusion near a (110)<111> dislocation core, the intention being to extract mechanisms that can be fed into kinetic Monte Carlo simulations of climb. We will present results on binding and migration activation of the single vacancy as a function of distance from the core, along with evidence showing the adparticle nature of binding of additional vacancies. We then build upon this understanding to discuss results on the migration energetics of the additional vacancies relative to that of the single vacancy migration. From these results we obtain a general set of self-consistent observations on vacancy-core binding, and discuss their applicability in a kinetic Monte Carlo simulation framework.

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Preference: Oral Presentation

Presenter: Timothy Lau

¹ T. T. Lau, C. J. Först, X. Lin, et al., Physical Review Letters **98**, 215501 (2007).

[NOTE: I would like this abstract to be considered for the travel fellowship.]

In situ study of the evolution of dislocation structures during strain path changes

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During plastic deformation of metals, such as copper, dislocations are produced, and as the dislocation density increases their arrangement becomes markedly heterogeneous. A structure is formed, consisting of almost dislocation free regions separated by dislocation rich boundaries. This structure changes as the deformation proceeds leading to progressively smaller boundary spacings.

At the APS synchrotron we have set up a novel X-ray diffraction technique, which combines an angular resolution of 5 millidegrees with fast three-dimensional reciprocal space mapping. This allows us to see reflections from deeply embedded dislocation free volumes and study the evolution of dislocation structures in polycrystalline copper samples during strain path changes. During a strain path change, the main axes of the deformation are altered, and the dislocation structure established during pre-deformation may become unstable and be replaced by a new structure characteristic of the new deformation conditions.

The strain path changes considered are tension-tension sequences. Polycrystalline copper sheets are pre-deformed in tension to 5% strain and tensile specimen are cut with varying angles between the first and second loading axis. The second tensile deformation up to additional 5% strain is performed in situ while mapping a selected X-ray reflection of one particular bulk grain with high angular resolution. In this way, we are able to establish a systematic correlation between changes in the dislocation structure and the degree of the strain path change.

Preference: Oral presentation

Presenter: Christian Wejdemann

Crackling Plasticity

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As suggested by its very name and by smooth macroscopic stress-strain or creep curves, the classical view of plastic “flow” in crystalline materials is that of a smooth and homogeneous process. Yet, intermittency of plastic activity has been known for a long period of time. For example, it was described in Zn single crystals as early as 1932. However, these observations remained marginal, as the observed fluctuations were seen as sufficiently small and independent of one another to add at random to a smooth overall response. A fundamentally different picture emerged during the last few years, that of a scale-free intermittent plastic activity characterized by power law distributions of dislocation avalanche sizes, time correlations and aftershock triggering as well as fractal patterns and complex space-time coupling. First experimental evidences came from acoustic emission (AE) experiments on deformed ice single crystals that showed power law distributions of AE amplitude and energy, where the maximum AE amplitude A_0 of an event is a proxy of the strain increment carried by the avalanche. These results were first presented to the dislocation community at *Dislocations2000*. Since then, they have been supported by different modelling approaches including 2D and 3D discrete dislocation dynamics, phase-field or continuum models. Independent experimental support was obtained from compression tests on Ni micron-size single crystals that showed staircase-like stress-strain curves with power law distribution of step size.

All of these findings argue for a renewed viewpoint on crystalline plasticity, reminiscent of the concept of crackling noise describing out-of-equilibrium physical systems with bursts of activity (avalanches), in close vicinity to criticality. Recent monitoring of the plastic deformation of metallic single crystals (Cu, Zn, Cd) from AE and micro-extensometry revealed the universal character for such intermittent plasticity: extreme fluctuations appear to be the rule, not the exception. We note however that (i) the existence of an internal length scale in polycrystals, the average grain size, limits the amplitude of fluctuations and therefore breaks down the scale invariance, and that (ii) there are still doubts on whether this critical dynamics develops in materials with low dislocation mobility (because of e.g. high lattice friction), when obstacles to dislocation motion (such as Peierls barriers, microparticles) either hinder or slow down free rearrangements of the dislocation population.

In this presentation, I will review the story of this “crackling plasticity” since *Dislocations2000*, and will discuss its consequences in terms of modelling of plastic deformation.

Dislocation dynamics, mean free path and slip avalanches in fcc crystals

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At the micrometer scale, plastic deformation happens by intermittent bursts or slip avalanches, which are characterized by scale-free behavior within a bounded domain of amplitudes or energies. The probability density of slip avalanches, their processes of initiation and termination and their contribution to dislocation storage during plastic flow are investigated with dislocation dynamics (DD) simulations. For this purpose, a representative volume element of copper with periodic boundary conditions is strained along high symmetry orientations. The distribution of avalanches measured with DD simulations exhibits, for all the tested orientations, a scaling exponent of 1.6 similar to what is reported in the literature. However, the corresponding average amplitude is found to be orientation-dependent. Furthermore, for all tested orientations, the ratio of the dislocations mean free path, as defined in continuum plasticity models, to the average characteristic length traveled by dislocations during slip avalanches appears to be a constant. This constant ratio shows that an implicit coarse-graining procedure is performed when measuring dislocation mean free path in DD simulations or consistently that the discrete nature of plastic deformation in fcc crystals can be incorporated into continuum models.

Statistical Characterization of Dislocation Systems with Dislocation Dynamics Simulation

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The usual goal of performing Discrete Dislocation Dynamics (DDD) simulations is to study the microscopic phenomenology of bulk or microcrystal deformation. Here we present another utilization of the DDD methodology, to provide input to statistical theories of crystal plasticity.

The last ten years saw the steady development of continuum bulk crystal plasticity theories based on the statistical mechanics of many-dislocation systems. One of the most important findings in strongly simplified two-dimensional slip geometries was the recognition that gradient terms, needed to describe size effects in continuum theories, are the direct consequences of short-range dislocation correlations. With the advent of three-dimensional generalizations of these continuum plasticity theories it became necessary to study the pair correlation functions of the complete three-dimensional dislocation problem. In this paper we present DDD simulation results for the range of dislocation pair correlations in fcc single crystals.

Recently, the intermittent plastic deformation of microcrystals has attracted a lot of interest. As typical for critical phenomena in general, many observed statistical characters of microcrystal plasticity show scale-free characteristics. Experimental results for the probability distribution of strain burst sizes also fall into this category, which would paradoxically indicate the largest strain bursts to be observable in macroscopic samples. With the DDD simulation of the quasi-static plastic deformation of a large number of fcc microcrystals we established the existence of an upper cut-off for the scale-free distribution of strain burst sizes. By varying the system size, the slip geometry, the temperature and the loading conditions, a universal functional form for the strain burst size distribution function was also demonstrated for a wide range of different conditions.

Preference: Oral presentation

Presenter: Ferenc F. Csikor

Topology and transport in driven vortex lattices

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PACS numbers: 74.25.Qt, 61.72.Mm

Recent studies have established a tight connection between driven vortex lattices in Type II superconductors and plastically deforming crystals. Both the atomistic and the mesoscopic behavior of disordered vortex assemblies under the effect of applied external currents implies topological rearrangements which involve dislocations and dislocation assemblies and result in the emergence of polycrystalline and amorphous states.

In this work we would like to emphasize the close relation between topological adjustments of the vortex lattice and its electrodynamic response. We perform a numerical study of the critical current by tuning certain relevant parameters, namely the magnetic field, the density of defects and, most importantly, the typical disorder strength, or pinning force.

In the case of weak pinning interactions, the dynamics of dislocation assemblies is the relevant mechanism that accounts for the collective motion of the vortex array. Dislocations rearrange into grain boundaries, accounting for the emergence of polycrystalline order. We prove that grain boundary interactions with defects are responsible for a non-trivial dependence of critical currents on the average defect density and we are able to corroborate previous analytical results which predicted the observation of individual and collective pinning regimes. Dislocation motion is associated with non trivial $1/f$ -noise features, which signal the emergence of correlated deformation patterns and strain avalanches.

In the case of higher defect strengths, instead, the vortex assembly loses lattice ordering and falls into a completely disordered phase. The consequent increase in the number of degrees of freedom results in a huge increase of the critical current. Depinning is now strongly heterogeneous, accompanied by a sharply discontinuous transition and jerky individual vortex dynamics. For applied currents right above the depinning threshold, the flowing state is anticipated by a moving state in which only a restricted number of vortices is in motion and plastic activity is strongly localized.

Preference: Oral presentation

Presenter: Paolo Moretti

Evolution of Dislocation Patterns in FCC Metals

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Dislocation patterning in fcc metals following plastic deformation has been extensively investigated using transmission electron microscopy. Although FCC metals form similar dislocation patterns following plastic deformation, the arrangement of dislocations into different patterns varies for each metal. These differences are believed to emanate from metallurgical factors and deformation process variables.

In order to correlate between dislocation patterns and different metallurgical parameters we performed systematic compression experiments in pure polycrystalline aluminum, nickel, copper and gold at room temperature.

Al, Ni, Cu and Au form a cellular structure. With increasing strain the dislocations within the cell's boundaries tend to rearrange themselves into ordered arrays. The main differences between those metals are in the strain necessary for the dislocations to rearrange themselves.

The rearrangement of the dislocations within the boundaries depends mainly on the ability of dislocations to cross slip, where the activation energy for cross slip is proportional to G^2/γ (G - Shear modulus, γ - stacking fault energy).

In this work we scale the dislocation patterning of similar fcc metals according to their activation energy to cross slip.

We have found that above a minimum strain (Al- 10%, Au- 30%, Ni- 40%, Cu- 50%), the dislocations rearrange themselves within the DBs. As expected, Al, with the lowest activation energy for cross slip and the highest homologous temperature, forms arrays of ordered dislocation at the lowest strain. Copper, having the highest activation energy and medium homologous temperature requires the highest strain between the four metals.

The strain required for the rearrangement of the dislocations in Au and Ni was found to be similar, having mid values between those of Al and Cu, since their activation energies are similar. Nevertheless, the dislocations rearrangement in Au requires a lower strain, since the homologous temperature of Au is higher than that of Ni.

2 - Dimensional Dislocation Dynamics Models of the Brittle-Ductile Transition in Body-Centred Cubic Metals

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Abstract

Dislocation-dynamics simulations of the crack-tip plasticity and resultant shielding of the crack tip have been developed to model the brittle-ductile transition (BDT), and have been applied to model the BDT in iron and in tungsten. The modelling has been closely associated with experimental studies of the BDT in single-crystal and poly-crystalline specimens of these materials.

The simulations use a simple model of the crack-tip plastic zone as two $\{101\}$ slip planes, symmetrically disposed about the crack tip ($[100]$ crack front with a (010) crack plane), with a single dislocation source on each plane. The models simulate the real loading rates, etc. used in the experiments. Modelling was performed using two different variants of the dislocation velocity / stress / temperature relation; one empirically based one, and one based on the fundamental double-kink mechanics of screw dislocation motion. Results from both variants are very similar, as the dislocations self-organise in the developing plastic zones, to give a constant internal stress at which the two velocity laws are approximately equivalent. The effect of the emitted dislocations on the crack tip stress field (“shielding”) is tracked by the model; fracture is assumed to occur if the crack-tip stress intensity factor reaches the “Griffith” (pure cleavage) fracture toughness of the material.

The models predict, for the first time for a dislocation-based approach, an explicit brittle-ductile transition; above a critical temperature, dislocation shielding is such that the crack-tip stress intensity factor never reaches the fracture toughness. Predictions of the models give a good *quantitative* fit to the experimental transition temperatures.

Dislocation dynamical modelling of the ductile-brittle-transition

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Reactor pressure vessel steels exhibit a strong temperature dependence of their toughness. Fracture at sufficiently low temperatures occurs by cleavage in an unstable manner with little energy absorption, while at higher temperatures ductile failure accompanied by considerable energy absorption is observed. The transition between these different fracture modes is affected by dynamic interactions between dislocations and the inhomogeneous stress fields of notches and small cracks. In the present work a dislocation dynamical model for the ductile-brittle-transition (DBT) is proposed, which takes those interactions into account. The model includes blunting and stress-triaxiality, which are found to be dynamically coupled. The evaluation of the model gives a simple, general criterion for the DBT as well as an explanation of the increase of toughness in the quasi-brittle regime. Furthermore the different levels of scatter of toughness data in the quasi-brittle and the transition regime can be understood. The influence of irradiation-induced changes in the plastic flow properties on the DBT is discussed and related to the DBT temperature shift. Moreover, as the model is dynamic in nature, it gives a natural explanation of the observed rate dependence of fracture toughness.

RESEARCH IN MECHANICS AND MATERIALS*

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According to Leonardo da Vinci, mechanics is the paradise of mathematical sciences. Mechanics and materials, pervasive and over-arching in all disciplines, are really two sides of a coin, very rich in their interfaces and rewarding areas for research. Nanotechnology is the creation of new materials, devices and systems at the molecular level – phenomena associated with atomic and molecular interactions strongly influence macroscopic material properties with significantly improved mechanical, optical, chemical, electrical and other properties. Nobelist Richard Feynman back in 1959 had the foresight to indicate, “there is plenty of room at the bottom”. Former National Science Foundation Director Rita Colwell in 2002 declared, “nanoscale technology will have an impact equal to the Industrial Revolution”. The transcendent technologies and transformative research include nanotechnology, microelectronics, information technology and biotechnology. These technologies are the primary drivers of the twenty first century and the new economy. Mechanics and materials are essential elements in all of the transcendent technologies. Examples of research opportunities, education and challenges in mechanics and materials, including experimental, numerical and analytical methods, simulation-based engineering and sciences, fracture, dislocations, nanomechanics, carbon nano-tubes, bio-inspired materials, as well as improved engineering and design of materials are to be presented and discussed.

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* Opinions expressed are those of the author’s, not necessary those of the National Science Foundation.

Irreversible Thermodynamics Modelling of Plastic Deformation over Wide Ranges of Strain Rates

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Abstract

Irreversible thermodynamics has been employed successfully to describe the dislocation density evolution during plastic deformation of metals at low strain rates [Huang et al. Mater. Sci. Tech. 23 (2007) 1105, Huang et al. Mater. Sci. Tech. (2008) accepted]. The present work extends the irreversible thermodynamics approach by accounting for phonon and electron drag effects. A general dislocation evolution equation is derived for wide ranges of strain rates. It is found that there is a transitional strain rate ($\sim 10^3 \text{ s}^{-1}$) over which the phonon and electron drag effects play a dominant role in dislocation accumulation resulting in an important raise in the dislocation density and flow stress. It is interesting to note that the current model reduces to the classical Kocks-Mecking model at low strain rates. The model is applied to pure Cu deformed at room temperature and at strain rates ranging from 10^{-4} to 10^4 s^{-1} showing good agreement with experiments.

Preference: Oral presentation
Presenter: Mingxin Huang

In-situ Deformation Experiments: Insights in Small Scale Plasticity

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In-situ deformation experiments of miniaturized materials provide the advantage of observing the plastic behavior during loading. As a consequence stress-strain data may be directly interpreted based on the observed deformation mechanisms. E.g. recent tensile testing of polycrystalline Cu wires with diameters of 10 to 50 μm revealed load drops when glide bands in individual Cu grains became visible (Fig.1). A similarly behavior was noticed during tensile straining of single crystalline Cu samples with diameters down to about 1 μm inside an SEM. In agreement with that, localized dislocation bursts have been observed by in-situ TEM straining experiments of thin metal films with film thickness below 1 μm .

Comparing the flow stresses of e.g. Cu across the length scales with critical dimensions ranging from 50 μm down to 0.2 μm reveals that at the smallest dimensions the size dependent flow stresses are influenced by dislocation nucleation. This is also supported by TEM straining results of thin single-crystalline metal films. The results will be critically discussed.

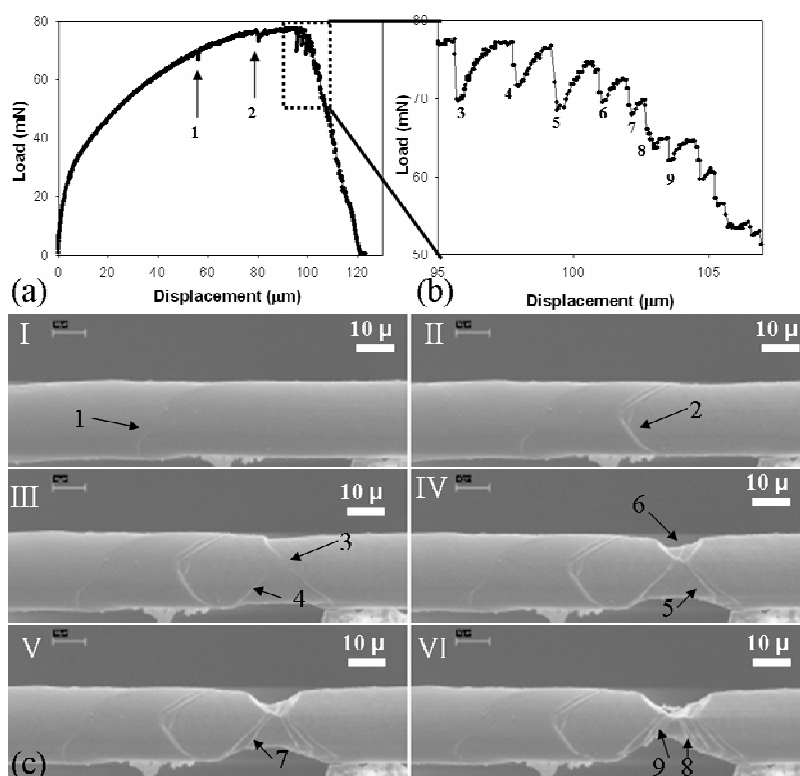


Fig.1: Tensile curve (a,b) and sequential in-situ SEM images (c) of an as-annealed 25 μm Cu wire. From B. Yang (Leoben), unpublished.

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Determination of Geometrically Necessary Dislocations Distributions using Electron Backscatter Diffraction

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Electron back scatter diffraction (EBSD) is a key quantitative microstructural analysis technique available on scanning electron microscopes. Hough transform based analysis is used for automated crystal orientation mapping at an angular resolution of $\sim 10^{-2}$ rads ($\sim 0.5^\circ$). Recently we have dramatically improved the angular sensitivity to $\sim \pm 10^{-4}$ rads by using a cross-correlation based analysis. This allows small lattice rotations and even elastic strains to be mapped at nanoscale resolutions. The EBSD methodology will be briefly described.

The relationship between the distribution of geometrically necessary dislocations (GNDs) and the lattice curvature has been elegantly described by Nye through his dislocation tensor. Differentiation of the EBSD measured rotation field generates some of the lattice curvature terms that can be linked to a GND distribution through Nye's analysis. Currently EBSD measurements are undertaken on the sample surface so the variation of rotations with depth are not known (ie we have access to 6 of 9 lattice curvature terms).

Rotations and strains were measured near Berkovich indents made to depths of 0.5 μm , 1 μm and 2 μm within the interior of a large grain of polycrystalline iron. The crystal was not in any 'special' orientation with respect to the indenter. There is a clear scaling of the lattice curvature and hence GND content with the reciprocal of the indent depth in line with theory.

The method was used to examine plastic zones formed at pre-cracks in single crystal vanadium samples tested to failure in bending at different temperatures across the ductile-brittle regime. Plastic zones were markedly more extensive for the higher temperature tests for which higher K_{IC} values were recorded. A fatigue crack tip grown at elevated temperature in a single crystal superalloy was also studied. The plastic zone is clearly revealed and distinction can be made between the outer monotonic zone and inner cyclic zone. For both Vanadium and superalloy samples the in plane rotations are dominant in accord with expectations given the symmetry of the crystal and loading conditions.

Dislocation Source-Controlled Plasticity in FCC Micropillars: Recent Experiments and Modeling Using the Line Tension Approximation

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Recent experiments have shown that FCC single crystals in the micrometer size range show significant size effects, with smaller being stronger, even when the crystals have little initial microstructure and are tested in uniaxial compression with no significant gradients of strain. These size effects suggest that plasticity is dislocation source-controlled, wherein smaller volumes are stronger because fewer sources of dislocations are available. The evidence for source-controlled plasticity is reviewed and recent attempts to describe the corresponding size effects on strength are described. One central idea is that for very small crystals dislocations leave the crystal more frequently than they multiply, by processes such as double cross-slip, forcing other, harder, sources of dislocations to be activated. In the extreme, dislocations have to be nucleated either at the surface or in the bulk of the crystal, which requires very high stresses. Support for this picture is provided by recent in situ TEM observations on nickel pillars showing that in some cases *all* of the dislocations initially present in the pillars escape from the crystal during deformation, leaving it completely free of dislocations. Recent computational modeling also supports the idea that the high strengths of single crystal micropillars may be associated with dislocation starvation and source-controlled plasticity. It is suggested that dislocation dynamics modeling using the line tension approximation may allow some of the key dislocation processes in micropillars to be described. It is shown that dislocations extending across thin crystal slabs can be modeled quite accurately using the line tension approximation, suggesting that extension of this approach to micropillars might be useful. Advantages and disadvantages of using the line tension approximation in DD modeling plastic deformation of thin slabs and pillars will be described.

Smaller is stronger: a view obtained by in-situ Laue diffraction

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Plasticity in single crystal micron sized pillars has gained considerable interest since the development of the micro compression technique and the observation of a “smaller is stronger” effect with decreasing pillar diameter. Plastic deformation is often observed as individual slip events that are reflected in discrete strain bursts. Large scattering among the data is reported, where pillars of similar orientation deform according to different slip systems, sometimes shearing-off or barrelling. To address the scattering amongst the data and to understand the mechanism behind the increase in strength in terms of existing or new theories, one needs information on the microstructural details of the sample before, during and after deformation.

An in-situ micro compression device has been developed at the Swiss Light Source (SLS) allowing for the continuous measurement of time-resolved white beam Laue diffraction patterns during compression of micron-sized pillars, that captures the initial microstructure and the changes in microstructure during deformation. Former measurements have for instance demonstrated the presence of initial strain gradients and their role on the deformation mechanisms activated during compression (PRL, 99(2007)145505) or evidenced classical type-II hardening in spite of higher yield stresses (APL 92(2008) 71905). On the other hand, Laue analysis also evidenced for some pillars the presence of microstructural characteristics (such as a low angle grain boundary) precluding them from the realm of single crystal plasticity and thus allowing for a reduction of the scatter among measurements, since these pillars no longer belong to the domain of the statistically unknown (APL 91(2007)131909). Here we present a new series of in-situ Laue diffraction experiments performed on Cu, Ni, Au and Al pillars with diameters between 1 to 10 micron, made in different laboratories, using different FIB procedures. The results emphasize (1) microstructural defects that do not belong to the single crystal domain, (2) evolution of the microstructure during compression evidencing the complex boundary conditions of a micro-compression technique, and (3) the increase in strength when the pillar diameter gets smaller. The results will be discussed in terms of existing and new developing theories addressing “smaller is stronger”.

Statistical Description of the Intermittent Plasticity and Creep of Micron-sized Crystal Pillars

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There is increasing evidence that crystal plasticity is jerky – the apparently smooth plastic curve of a bulk crystalline material actually consists of nanometer-sized bursts, as shown by acoustic measurements on ice (Weiss, Miguel and co-workers). In the case of bulk crystals, the jerky flow may not be very important for applications such as manufacturing, because the burst sizes are minute compared with the specimen size (i.e. the burst strains are vanishingly small). However, recent compression experiments on crystalline specimens of micron or sub-micron dimensions also reveal that their flow behaviour is jerky, and in this case the burst strains are large, typically up to a few % for one burst. A smooth, power-law type of plastic curve is therefore inappropriate for such a situation – the plasticity of such small crystals simply needs another description.

In this work, we first present experimental results on micron and submicron-sized aluminium columns, fabricated by focused-ion beam milling, which were subjected to compression in a nanoindenter using a flat-ended tip to reveal their deformation behavior. Close examination of the jerky flow curves of these columns shows, as other researchers have observed in other systems, that the deformation consists of quick bursts separated by elastic segments. *Post mortem* transmission electron microscopy investigation of the columns revealed that their dislocation density did not grow significantly after severe deformation. This is an important finding which indicates that each burst is completed with insignificant accumulation of residual dislocations in the sample. The apparent “strain-hardening” behaviour is therefore completely different from that in a bulk crystal where dislocations cannot escape and have to interact, to produce the Taylor-type of hardening effect. Instead in a micro-column, the so-called “strain-hardening” is simply a manifestation of the burst-elastic behaviour where the bursts are stochastic, and more or less independent, events. Under compression at constant loads, the aluminium columns creep also by the emission of intermittent strain bursts. The burst emission frequency drops as time proceeds, and emission eventually stops for very long load-holding times.

Based on the above observations, a Monte Carlo model is proposed in this work to describe the stochastic and jerky nature of deformation of these micro-columns. The input to this model includes the probability of occurrence of the bursts in their sequential order, and the size distribution of the bursts as a function of stress. Both are experimentally determinable information and the model can predict other deformation characteristics such as the stress-strain curve (i.e. the apparent strain-hardening behaviour) and its statistical spread, the overall burst size distribution, etc. Agreement with experiments under both load-ramp and constant-load conditions is good, indicating that the model provides a valid description for the intermittent deformation of micron-sized crystals.

Discrete dislocation dynamics study of the mechanical properties of micro-samples

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The increasing use of MEMS requires a better comprehension of the mechanical properties of metallic structures in the micro-meter range. Therefore, dedicated experiments on thin films or single crystalline samples can be found in the literature. In these experiments, e.g. compression tests on single crystalline sub-micron and micro-pillars have shown that the flow stress is size-dependent, where a decrease in the pillar diameter is correlated to an increasing average flow stress and an increasing standard deviation of the flow stress. More recently, tension tests on Cu wires have revealed an aspect ratio dependency of the size effect and in the hardening behavior of thin wires.

In this presentation, three dimensional discrete dislocation dynamics simulations of wires with various aspect ratios are presented. Most simulations were performed starting from preexisting FR sources with random orientation and prescribed length interval for the sources. The mechanical properties of the micro-samples under uniaxial loading in single and multi slip orientations are simulated and analyzed.

The simulation result coincide with the experimental trend that smaller is stronger, and for an aspect ratio of sample length to width of 2 to 1, we obtain a power law exponent of about -0.6 for the flow stress as a function of the width of the sample [1]. The important role of the evolving dislocation microstructure for the deformation behavior for different pillar sizes will be presented [1]. Also, the dislocation dynamics results indicate that the aspect ratio of the micro-samples influences the flow stress of the pillars, most pronounced for smallest diameter.

The simulation results will be discussed with respect to different explanations for the size effect, such as dislocation starvation, assuming that dislocations escape through the surface more easily in smaller volumes than in larger ones, or the truncation model for dislocation sources close to surfaces, or the role of dislocation multiplication and source formation in confined volumes.

[1] Senger J, Weygand D, Gumbsch P, Kraft O; Scripta Materialia; 58 (2008) 587

Preference: Oral Presentation

Presenter: Jochen Senger

Title: Dislocation Dynamics and Plasticity in FCC and BCC Single Crystal Micro-Pillars
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Recent experiments on the compression of single crystal micropillars show a dramatic increase of flow stress when the pillar diameter decreases below one micron. These experiments also present an interesting opportunity to quantitatively compare theoretical models of defect dynamics with the measurable mechanical properties of a crystal. In the widely discussed dislocation-starvation model, the observed size effect is explained in terms of the need for continued nucleation of dislocations (such as from the surface) since they escape easily through the surface of the micropillar. Through a combination of Molecular Dynamics and Dislocation Dynamics simulations, we found that a freshly nucleated dislocation in BCC pillars self-replicates before exiting the crystal (but not in FCC pillars). The process can repeat itself so that a single nucleation event can lead to a significant amount of plastic deformation. Due to this self-replication mechanism, a BCC pillar is less likely to be dislocation-starved compared to an FCC pillar of the same size. The fundamental mechanism of this process is explained. Consequences of this mechanism on the size effect and the possibility of experimental verification are discussed.

***IN-SITU* NANOCOMPRESSION OF GUM METAL PILLARS**

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Abstract

Gum Metal describes a newly developed set of alloys with nominal composition Ti-24(Nb+V+Ta)-(Zr,Hf)-O. In the cold-worked condition these alloys have exceptional elastic elongation and high strength; the available evidence suggests that they do not yield until the applied stress approaches the ideal strength of the alloy, and then deform by mechanisms that do not involve conventional crystal dislocations. To clarify the mechanisms involved, *in situ* microcompression experiments were performed in a TEM on sub-micron sized pillars fabricated with a focused-ion beam. Results from these tests on solution-treated and cold-worked specimens were compared with TEM observations after *ex situ* nanoindentation, which revealed unusual patterns in the pits of the indents. Current findings suggest two stages of deformation starting with dislocation motion in the solution-treated condition, which develops into an unidentified mechanism in the cold-worked alloy.

Athermal mechanisms of size-dependent crystal flow gleaned from three-dimensional discrete dislocation simulations

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ABSTRACT

Recent experimental studies discovered that micrometer-scale face-centered cubic crystals show strong strengthening effects, even at high initial dislocation densities. We use large-scale 3-D discrete dislocation simulations (DDS) to explicitly model the deformation behavior of FCC Ni microcrystals in the size range 0.5 – 20 μm . The study shows that two size-sensitive athermal hardening processes, beyond forest hardening, are *sufficient* to develop the dimensional scaling of the flow stress, stochastic stress variation, flow intermittency and, high initial strain-hardening rates, similar to experimental observations for various materials. One mechanism, source-truncation hardening, is especially potent in micrometer-scale volumes. A second mechanism, termed exhaustion hardening, results from a break-down of the mean-field conditions for forest hardening in small volumes, thus biasing the statistics of ordinary dislocation processes.

Pillar Plasticity: 2.5D Dislocation Dynamics Simulations

Authors: A. Amine Benzerga and P.J. Guruprasad

Compression of micro- and nano-pillars of various crystalline materials has revealed significant size effects on their plastic behavior. Here, we report on a theoretical investigation of plasticity size effects in the absence of macroscopic gradients in the applied loading. Extensive computations are carried out, which are based on the framework of mechanism-based discrete dislocation plasticity. For computational efficiency, the 2.5D dislocation dynamics (DD) paradigm is used whereby key three-dimensional, short-range dislocation interactions are incorporated through a set of constitutive rules in a plane strain representation of the dislocations. The effects of specimen diameter and initial dislocation density are explored with the former varying from hundreds of nanometers to tens of microns and the latter spanning over two orders of magnitude. For low initial dislocation density, the pre-existing dislocation structure is found to affect the yield strength; some exhaustion hardening emerges which decreases in rate with increasing stress and unloading is purely elastic. For very high initial dislocation density, the 2.5D DD calculations predict a significant size effect on flow stress and work-hardening, which are both associated with the evolving, and not pre-existing, dislocation structure. A significant Bauschinger effect is also noted. For intermediate initial dislocation densities, more recent computations indicate a size effect on work-hardening with little or no Bauschinger effect. The plasticity size effect in the intermediate to high dislocation density regimes is explained in terms of an evolving effective GND density, which is quantified in the DD simulations. As a closure, a phenomenological plasticity model is developed which mimics the overall behavior of specimens of various sizes simulated with 2.5D DD.

In-situ Investigation of Nano-scale Plasticity in FCC and BCC Crystals via Homogeneous Deformation of Nano-Pillars.

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Abstract

Mechanical behavior of crystals is dictated by dislocation motion in response to applied force. To investigate plasticity under homogeneous deformation we developed micro-deformation methodology where nanopillars fabricated by Focused Ion Beam are uniaxially deformed and stress vs. strain relationship is obtained. Plastic flow stress increases according to power law as pillar diameter is decreased demonstrating that size effect exists even without strain gradients present in bending and indentation experiments. To visualize deformation we built a new instrument, SEMentor, with in-situ visualization capabilities, which measures mechanical response of nanoscale materials while capturing video frames. We present results of in-situ deformation tests and report mechanical strengths of pristine FCC and BCC nanopillars. All crystals show significant increase in flow stress with decreasing diameter in power-law fashion, but with different slopes. Microstructural and statistical analyses are also presented.

Dislocation source activation approach to explain size effects on plasticity in ultra thin metallic films of different microstructure

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The plasticity of metals exhibits a particularly strong size effect. As a consequence, flow stresses for metallic thin films and nanostructures have been repeatedly found to be significantly higher than in corresponding bulk materials and increase with decreasing dimension. However, the understanding of the underlying mechanisms is still incomplete. Here, we present a unified dislocation source activation approach capable to explain the experimental results of thin film systems with very different microstructure. Nanocrystalline (grain size of 10 to 30 nm) as well as single-crystalline and polycrystalline metallic films (20 to 1000 nm thick) with and without passivation have been tested by novel synchrotron-based tensile testing techniques under very similar conditions. It is found that the mechanical properties strongly depend on film thickness, grain size and interfacial properties. The analysis of the X-ray diffraction patterns as well as parallel careful microstructural characterization give new insight in the initial and evolving microstructure of the films. By considering all microstructural parameters and a change in deformation mechanism from full to partial dislocations for grains sizes or film thicknesses smaller than 100 nm, the scaling behavior of the flow stress can be described correctly for all film systems by a modified dislocation source model where the activation stress for single dislocations very likely governs the behavior.

Extended dislocations and dislocation reactions in $L1_2$ ordered superalloys

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Dislocation core structures and the effective γ -surface in $L1_2$ Ni₃Al have been evaluated by atomistic modelling using EAM potential by Y. Mishin [1].

Using atomistic modelling we analysed thoroughly various dissociation reactions of perfect superdislocations in $L1_2$ Ni₃Al on the basis of the configuration of dislocation core splitting and structure of the regions separating partials. The results of $\langle 110 \rangle \{111\}$ and $\langle 112 \rangle \{111\}$ extended dislocations simulations are compared with TEM observations of these dislocations in single crystal superalloys subjected to creep testing.

The well-known γ -surface concept suggested by V. Vittek [2] has been extended to the case of the shift of one part of the crystal with respect to another in two adjacent (111) planes of the stacking fault. The study of the obtained effective γ -surface showed existence of five stable planar faults, namely superlattice intrinsic stacking fault (SISF), superlattice extrinsic stacking fault (SESF) that can be treated as SISF over SISF, antiphase boundary (APB), complex stacking fault (CSF) and CSF over SISF. The existence of last faulted configuration has never been reported before. Comparison of the effective γ -surface with the conventional one is conducted and the implications of the obtained results for dislocation dissociation are then considered.

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Preference: Oral presentation

Presenter: R. E. V oskoboinikov

How metallic thin films on substrate accommodate or resist plastic deformation : The contribution of *in situ* TEM experiments.

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Size effects in materials science are drawing a great deal of attention from the scientific community because they question the limits of the dislocation theory. Thin metallic films on substrates exhibit a large resistance to deformation, and in the micron range, this dependence scales linearly with the inverse of the thickness. Such a linear increase of the films strength has been rationalized in term of confined dislocation motion (Nix, [1]). In this fairly simple, and thus popular model, the yield stress of a metallic film on a rigid substrate is attained when threading dislocations start to shear the film, increasing simultaneously the length of interfacial dislocations in their wake. This model leads to the correct stress values for pseudo epitaxial metallic films (such as Al or Cu on sapphire) but falls significantly short when it comes to metallic films that possess an amorphous interface with the substrate (Al on oxidized Si for instance) [2]. Considering the image forces seen by the interfacial dislocations in both systems, the opposite effect should be observed.

In films thinner than about 200 nm, yield stress plateaus or even decreases, clearly calling for an alternate plastic relaxation mechanism. Parallel glide of dislocation, a potential symptom of enhanced grain boundary diffusion, is one of the possible substitution process, but so far, it has never been observed elsewhere than in Cu films [3].

Here, we will show that *in situ* TEM can display the dislocation mechanisms while they operate in thin films and thus directly corroborate or contradict existing theories. For thicker films, amorphous interfaces play the role of dislocations sinks, similarly to free surfaces [4]. The increased strength of metallic films with such amorphous interfaces is thus dictated by the ability to create fresh dislocations rather than propagating them. In thinner films, diffusion processes are clearly at work, but harder to display [5]. Finally, and similarly to what has been recently observed in nanocrystalline metals, plasticity can also be carried out by grain boundary displacements [6]. The driving force for this flow of matter from small precipitates to larger ones is their Gibbs free energy. We will show that one can calculate rather directly the diffusivity of the dislocation from such dynamic experiments. Even if potential artifacts such as local stress, presence of free surfaces and surface energy values of Si particles are taken in account, the method leads to a fairly precise measurement of the diffusion parameters. The pipe diffusivity is, as expected, orders of magnitude larger than its bulk counterpart. By repeating purposely the same experiments at different temperatures we were also able to determine the activation energy of pipe diffusion.

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Brittle and Ductile Failure of Si Nanowires in Tension, Torsion and Bending

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We performed Molecular Dynamics simulations of Si nanowires (NWs) with the modified embedded-atom-method (MEAM) potential under uniaxial tensile loading at a constant strain rate until failure. We found that the brittle or ductile fracture behavior of the NWs depends not only on the temperature but also on the NW diameter. Surprisingly, NWs with diameter less than 4 nm become ductile regardless of the temperature. A dislocation loop model is proposed to explain the size and temperature dependence of the observed fracture behavior. The prediction from these computer simulations are discussed in comparison with recent *in situ* tensile deformation of Si NWs.

While the intrinsic strength of NWs against tensile deformation can be conveniently modeled using periodic boundary conditions (PBC), modeling torsional and bending loading is challenging due to their incompatibility with PBC. We present a unified approach for atomistic modeling of torsion and bending of NWs by developing the torsional and bending periodic boundary conditions (t-PBC and b-PBC). Molecular Dynamics simulation of Si NWs under these boundary conditions exhibit several types of failure modes depending on their diameters.

Plasticity of nanocomposite wires during in-situ tensile tests under X-rays: size effect, Bauschinger effect and dislocation storage.

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Copper-based high strength nanocomposite wires are prepared by severe plastic deformation (Accumulative Drawing and Bundling process) for the windings of high pulsed magnets. The process leads to a multi-scale Cu matrix containing up to $N=85^4$ ($52.2 \cdot 10^6$) continuous parallel Nb filaments or tubes with diameter down to few tens nanometers. After heavy strain, the multiscale Cu matrix is nanostructured and the Nb reinforcing phase is strongly refined. The resulting macroscopic strength is in excess from rule of mixture predictions calculated from bulk coarse-grained counterparts: an ultimate tensile strength up to 2 GPa is reached at 77K.

In-situ tests have been performed under synchrotron beam on nanocomposite wires containing Nb nanotubes. The evolution of elastic strains and peak profiles versus applied stress evidences the co-deformation behavior with different elasto-plastic regimes: the Cu matrix exhibits size effect in the finest channels while the Nb nanotubes remain elastic up to the macroscopic failure, with a strong load transfer from the Cu matrix onto the Nb nanotubes. During multiple loading-unloading cycles, the macroscopic stress-strain curve evidences strong hysteresis that could be independently followed in the different phases via the measurement of elastic strains: internal stresses are building-up because of large yield stress mismatch in the nanocomposite structure. This Bauschinger effect can be related to the dislocation storage in the different phases (APL 90 (2007), 241907). The elasto-plastic transition is also studied in the different phases, in particular the microplastic to macroplastic transition with respect to microstructure size.

Electrical Properties of Dislocations in GaN

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The electrical conduction along dislocations in semiconductors has been one of the long-standing, controversial problems in the study of dislocations. In principle, dislocations in semiconductors are expected to form one-dimensional electronic states in the bandgap and to behave like quantum wires. However, only few examples of dislocation conduction have so far been confirmed experimentally and detailed conduction mechanisms have not been clarified yet. In this study, possible dislocation conduction has been investigated in GaN, which has attracted much attention in recent years for various applications including blue light emission diodes.

Single crystals of n-GaN were plastically deformed by compression test in Ar flow at 1223 K, and the plastic strains of 5 and 10 % were induced. TEM observations confirmed that dominantly edge dislocations have been introduced on the prismatic plane. Macroscopic electrical conductivities were measured along different directions by 2-probes method. Electrical conductivities along individual dislocations were microscopically investigated by a scanning spreading resistance microscopy (SSRM).

A large anisotropy was found in the macroscopic electrical conductivity measurements: the path across the slip plane showed a lower conductivity by a factor of about 10^4 than the path parallel to the slip plane. This can be explained by the formation of carrier depletion region around dislocations. The SSRM images exhibited highly-conductive spots of about 50 nm in diameter on the surface of the deformed samples. Because no such spots were observed in the undeformed sample and the density of the spots observed in the deformed samples is comparable to the introduced dislocation density, the highly conductive spots can be attributed to the dislocation-core conductivity.

Preference: Oral presentation

Presenter: Yasushi Kamimura

Dislocation self-organization in fcc metals deformed in single slip: the underlying microscopic manoeuvres

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It has been shown experimentally that dipolar annihilation is manifested in strings of edge or near-edge prismatic loops exhibiting a unique orientation relationship. String formation is, however, a rather complex dynamical process, difficult to apprehend from *post mortem* deformed samples. *In situ* TEM is of no help in this case. It has been predicted that the overall shape of the strings together with that of the individual loops forming the strings depend on the relative velocities of the approaching dipolar dislocations. The dd simulations presented in this paper support this view. They also demonstrate the great variety of situations that can be encountered in practice when the relative positions, characters and lengths of the sources that give rise to the dipole, are varied. dd simulations indicate that, if comprised of narrowly spaced loops, strings can act as a potent obstacle against dislocation motion, hence offering an explanation to the nucleation of dislocation entanglements. Various situations are shown and the limitations of this mechanism discussed.

Molecular dynamics simulations were undertaken to investigate the stability of loops versus full self-annihilation or collapse together with their resistance to being swept by mobile dislocations. The simulations were conducted in Al between 0K and 900K, with two different potentials and for dipoles heights comprised between 1 d_{111} and 10 d_{111} . Contrary to a common belief, edge dipoles neither collapse nor vanish. At low temperatures, for dipole heights of 5 d_{111} and beyond, dipoles exhibit the equilibrium configuration predicted by elasticity while, at high temperatures, they reorient to the 60  character to form the low energy faulted dipole configuration. For dipole heights of 4 d_{111} and below, a large variety of configurations is formed depending on both dipole height and temperature, including the above-mentioned 60  faulted dipoles. At very small heights, the dipole inner volume exhibits an array of ordered vacancies while at high temperatures it transforms into an alignment of stacking fault tetrahedra. In view of the limited simulation time achieved in MD, it cannot be ascertained though that SFT formation is limited to high temperature annealing. It is nevertheless clear that dipole annihilation does not clean up the crystal from its debris which remain obstacles to the passage of new dislocations, hence providing an alternative origin to the nucleation of entanglements.

Suzuki segregation

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Suzuki segregation is chemical segregation to a stacking fault, originally in an f.c.c. metal. Suzuki's^[1] interpretation involved regarding the stacking fault as a thin fillet of h.c.p. phase. We^[2] have examined segregation to stacking faults and twins in Cu-7at%Si at various temperatures. The results have been analysed on the basis of the Cu-Si phase diagram and do not support Suzuki's interpretation.

References

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STRAIN LOCALISATION IN POST-IRRADIATED METALS: TEM OBSERVATIONS, MOLECULAR DYNAMICS AND DISLOCATION DYNAMICS ANALYSIS

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ABSTRACT

Internal structural components in pressurized water nuclear reactors are exposed to irradiation, generating defect clusters in the form of interstitial Frank loops. This population of defects interacts with the development of plasticity and induces severe hardening and reduction of ductility. These macroscopic effects are usually ascribed to strain localization into microscopic shear bands, free of irradiation defect clusters. In this study, the formation of "clear bands" is examined in details, by combining Transmission Electron Microscopy observations (TEM) and numerical simulations, including Molecular Dynamics (MD) and Dislocation Dynamics (DD).

Hence, the atomic scale MD simulations helped to clarify:

- i- the nature of the interaction mechanisms between mobile dislocations and irradiation defect clusters, in a low stacking fault energy (SFE) metal,
- ii- the relative strength of the different possible dislocation/cluster configurations.

The TEM observations of deformed stainless steel specimens (at 350°C) after ion-irradiation indicate that:

- i- inside a clear band, a small fraction of the mobile dislocations absorb the defect clusters, become heavily jogged and eventually lose their initial mobility,
- ii- the rest of the mobile dislocations thus glide in a well formed clear band and for this reason, remain almost defect-free.

Information from MD results and TEM observations is then used to develop local constitutive rules for DD simulations, treating the dislocation/cluster interactions. The DD simulation volumes contain a realistic density of Frank loops. The simulation results provide an original clear band formation scenario, emphasizing the role of collective effects and jog transfer along the mobile dislocation lines. Interestingly, the characteristic dimensions of the simulated clear bands are consistent with the TEM observed ones, after ion-irradiation. This means saturation of the clear band thickness is obtained after gliding over a limited distance, i.e. no more than a few microns.

Preference: Oral presentation

Presenter: Christian Robertson

SUPPRESSING DISLOCATION GLIDE TO ACHIEVE IDEAL STRENGTH

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ABSTRACT

The maximum strength that can be realized in a material (ideal strength) is reached at the limit of elastic stability, that is, when the atomic bonds themselves become unstable with respect to shear or fracture. To achieve this limit in a metal it is necessary to employ some microstructural mechanism to pin potentially mobile dislocations until the ideal strength is reached. While this is a very challenging task, metallurgical criteria that may succeed in achieving it have been identified, and at least one example appears to have been achieved. If the composition of an alloy is adjusted so that its certain of its shear moduli approach zero, two simultaneous results are achieved: the ideal strength decreases to a relatively low value (which may still be large) and the efficiency of dislocation pinning by microstructural obstacles increases to the extent that very high critical shear stresses are reached at realistic obstacle separations. In this limit ideal strength becomes possible. An experimental example of this behavior appears to be realized in the “Gum Metal” alloys recently developed by Toyota R&D in Japan. These are bcc Ti-Nb-Zr-O alloys that have nearly vanishing moduli, and achieve strengths above 2 GPa with no apparent dislocation activity. Both theory and experimental observation suggest that dislocations are efficiently pinned in these materials until eventual shear failure at ideal strength.

Bridging atomic to continuum scale through thermodynamical analysis of molecular dynamics simulations: case of dislocation-void interaction

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Abstract

Given the time and length scales in Molecular Dynamics (MD) simulations of dislocation-defect interactions, MD results cannot be directly used in larger scale simulations or compared to experiment. A method is here proposed to extract from MD simulations fundamental quantities necessary to describe the interaction. The method is applied to determine the interaction energy, the critical local stress and the activation energy of the dislocation-void interaction as a function of temperature. It is shown how these parameters can be intuitively used in Dislocation Dynamics (DD) simulations in order to reproduce the interaction strength observed in MD simulations. First results show that the molecular statics simulations of dislocation-void interaction can be exactly reproduced by DD simulation. However, on the mesoscopic scale, thermal activation is found to enhance the stochasticity of the interaction while, at small void spacing and high deformation rate, the fluctuation of the void strength tends to vanish, in agreement with MD simulations.

Preference: Oral presentation

Presenter: Ghiath MONNET

Dislocation Observation in Protein Crystals by Synchrotron X-ray Topography

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Dislocations in protein crystals were veiled in mystery because of the long Burgers vectors (several nm). Recently, we have observed the clear dislocation images of lysozyme crystals that are one of typical protein crystals using monochromatic synchrotron white x-ray topography. The observed topographic images of dislocations were much clearer compared to those of any protein crystals that have been reported so far. It was demonstrated that millimeter-size crystals larger than extinction distance for X-ray topographic reflections are required to obtain clear images, that is, direct images for protein crystals. Straight, curved and loop-type dislocations were clearly resolved on the topographs. This indicates that dislocations observed in typical covalent and metal crystals can also be introduced even in protein crystals during the crystal growth.

Moreover, we have also observed mechanical properties of lysozyme crystals by a micro-hardness test. The protein crystals were clearly deformed and the slip lines appeared around the indentation mark. These slip lines corresponds to the trace of slip dislocations. We will discuss the relationship between grown-in dislocations and slip dislocations in the conference.

ATOMIC-SCALE MODELLING OF DISLOCATION INTERACTION WITH LOCALISED OBSTACLE

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and

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Abstract

Irradiation of metals with high-energy atomic particles creates nano-scale defect clusters, such as voids, dislocation loops, stacking-fault tetrahedra and irradiation-induced precipitates. They are obstacles to dislocation glide during plastic flow and give rise to hardening and, in some conditions, strain localisation. Approximations based on the elasticity theory of defects offer the simplest treatment of strengthening, but are deficient in many respects. Computer simulation has therefore been developed to provide atomic-scale detail of mechanisms and quantitative information on the influence of stress, strain rate and temperature. Recent results of modelling dislocations gliding under stress against obstacles in a variety of metals across a range of temperature are considered. The effects observed include obstacle cutting, absorption and drag. Simulations of 0K provide for direct comparison with results from continuum treatment of dislocations, and although some processes can be represented within the continuum approximation, others cannot.

Quantification of Solute Segregation at Dislocations

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One of the key parameters that influences the mobility of dislocations is the amount of solute segregation that is associated with the stress fields. Atom probe tomography has the necessary three-dimensional spatial and mass resolutions to quantify the extent and amount of solute segregation in the vicinity of dislocations for all elements. The relatively large volume of analysis and high data acquisition rate of the local electrode atom probe (LEAP[®]) enables the solute distribution around and along the core of dislocations to be quantified in materials with high dislocation densities. A wide field of view LEAP has been used to quantify level of solute segregation at dislocations in several neutron irradiated pressure vessel steels and model alloys. Examples of carbon-enriched Cottrell atmospheres, as well as the segregation of phosphorus and several other substitutional elements including silicon, nickel and manganese to dislocations will be presented.

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SOLUTE AND DISLOCATION JUNCTION INTERACTIONS

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ABSTRACT:

In this study, the role of solute segregation on the strength and the evolution behavior of dislocation junctions is studied by utilizing kinetic Monte Carlo and 3D dislocation dynamics simulations. The different solute concentrations and the character of the junctions are all included in the simulations in an effort to make a parametric investigation. The results indicate that the solutes have a profound effect on the strength of the junctions. Solute segregation can lead to both strengthening and weakening behavior depending upon the evolution of the dislocation junctions. The local solute concentration seems to be the more relevant parameter to characterizing the solute and dislocation interactions, due to the short-range stress field of solutes; and its bounds are set by the unconstrained volume dilatation.

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Atomistic simulations of dislocation-obstacle interactions

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The mechanisms of dislocation motion and dislocation – obstacle interaction are of practical importance to developing quantitative structure-property relations, mechanistic understanding of plastic flow localization, predictive models of mechanical behavior in irradiated metals and the dynamic response of materials to shock loading. Molecular dynamics simulations directly account for core interactions through semi-empirical interatomic potentials and provide fundamental insight into the sequence of events controlling dislocation migration and material deformation mechanisms. In this presentation, we describe our recent results to investigate the motion and interaction of screw, edge and mixed dislocations in fcc Cu, Al, Au, and Cu-Co alloys, and bcc Fe, Fe-Cu and Fe-Cr alloys. The simulations have been performed to investigate the dislocation interaction and detachment mechanisms with a variety of obstacles, including dislocation loops, stacking fault tetrahedra, voids and helium bubbles, as well as coherent precipitates, and reveal a number of unexpected results, including the Orowan looping of coherent precipitates. The atomistic modeling results are discussed in terms of developing theoretical expressions for obstacle strength and interaction rules for incorporating such obstacles into larger-length scale dislocation dynamics simulations, as well as comparing with available experimental results.

Non-Schmid plastic behavior and differences in slip activity in molybdenum and tungsten resulting from the core structure of screw dislocations

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Plastic deformation of BCC metals is controlled by $1/2\langle 111 \rangle$ screw dislocations. Their non-planar cores lead to very high Peierls stress and are also responsible for strong dependence of the yield stress on both the orientation of the Maximum Resolved Shear Stress Plane (MRSSP) and the shear stress perpendicular to the slip direction. The former reflects the so-called twinning-antitwinning asymmetry while the latter is entirely related to stress-induced transformations of the dislocation cores.

In this talk we present the results of our recent 0 K atomistic studies of the glide of $1/2\langle 111 \rangle$ screw dislocations in molybdenum and tungsten. The calculations were made using Bond Order Potentials that reflect the mixed metallic and covalent character of bonding in transition metals. The twinning-antitwinning asymmetry was found to be significant in molybdenum while it is negligible in tungsten. In contrast, the effect of the shear stresses perpendicular to the slip direction is much stronger in tungsten. Using these results we formulated 0 K yield criterion that captures the non-Schmid behavior resulting from the dislocation core effects. Using this criterion we identify the most operative $\{110\}\langle 111 \rangle$ system for uniaxial loadings with loading axes within the standard triangle. For tension this is always the most highly stressed $(\bar{1}01)[111]$ system in both molybdenum and tungsten. However, in compression a variety of slip systems become operative, depending on the orientation of the MRSSP. In molybdenum the $(\bar{1}01)[111]$ system is still primary for most orientations of the compressive axis but the tension/compression asymmetry is pronounced and principally governed by the effect of shear stresses perpendicular to the slip direction. Both these characteristics agree with experimental observations, which will be shown in this presentation. In tungsten the activity of the $(\bar{1}01)[111]$ system is much weaker and, instead, the low-stressed $(\bar{1}10)[111]$ system dominates. Unfortunately, no experimental data are available at present to verify this finding.

Preference: Oral presentation

Presenter: Roman Gröger

Dislocation Atomic Structures and Properties in Sapphire

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Low-dimensional structures, such as micro-clusters, quantum dots and one- (1D) or two-dimensional (2D) quantum wires, are of scientific and technological interest due to their unusual physical properties, which are quite different from those in the bulk. In this study, we show the successful results to fabricate “conductible 1D nano-wires bundle” inside an insulating ceramic single crystal by utilizing unidirectional dislocations. Sapphire (α -Al₂O₃ single crystal) was used as a model crystal. Firstly, high density of dislocations were introduced by mainly activating a primary slip system in sapphire using a two-stage deformation technique, and then plate specimens cut out from the deformed sapphire were annealed to straighten the dislocations. Thereafter, the plates, on which metallic Ti was evaporated, were heat-treated to diffuse Ti atoms inside sapphire. As a result, it was found that Ti atoms intensely segregated along the unidirectional dislocations within about 5 nm in diameter, indicating the formation of 1D Ti-enriched nano-wires in sapphire. Furthermore, the nano-wires were confirmed to have excellent electrical conductivity.

On the other hands, low angle grain boundary is known to consist of an array of dislocations. Recently, the studies concerning the low angle grain boundaries have been performed to study dislocation core structures in sapphire. It has been also found using high-resolution transmission electron microscopy (HRTEM) that the lattice dislocations in sapphire dissociate into partial dislocations. In this case, the boundary dislocations on low angle tilt grain boundaries dissociated into two partials dislocations with the narrow separation distance of a few nanometers and the separation distance decreased with increasing tilt angle. We'll show the method that the separation distance and dislocation periodicity can be controlled arbitrarily by controlling misorientation angle. This technique is also applied for fabricating the periodically located nano-wires. In addition, alumina bicrystals with low angle tilt boundaries including a slight twist component were fabricated using diffusion bonding technique, and then the resulting grain boundary structures were analyzed to investigate the structure transitions of boundary dislocations by a slight twist component.

Scaling constraints associated to plastic flow in nanograined polycrystals

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In these materials, the smallness of the grain size imposes very strong constraints on the mean free path of dislocations, their nucleation or multiplication rate, as well as on the respective activity of grain boundary (GB) sliding, GB migration, twinning and dislocation motion under the effect of an applied stress. It is now well established that the extent of the microplastic stage in these materials can be as large as 1%. This implies a critical analysis of the informations gathered from conventional measurement of fundamental quantities such as : the yield stress, the strain hardening rate, the strain rate sensitivity, and its relation with the activation volume. This communication develops a detailed analysis of the scaling constraints associated with the grain size, whose results are applied to the discussion of recent experimental results published in the literature.

On the core structure of dislocations in elemental semiconductors at high stresses

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After deformation at high pressure and low temperature it has been demonstrated using transmission electron microscopy (TEM) that dislocations with perfect core were nucleated in silicon at high stress, at temperature below the usual BDT temperature (see for example [1], [2]). Those dislocations are expected to be in the shuffle set, i.e. in the widely separated $\{111\}$ atomic glide planes as compared to the usual dissociated dislocations which are found in the glide set, the $\{111\}$ closest atomic planes. This is in agreement with previous calculations of Duesbery and Joos [3] on the double kink formation in silicon in this two possible atomic glide planes. From these observations, it can be postulated that dislocations with perfect shuffle core structure can pre exist to the nucleation to the usual dissociated dislocations found in silicon and that the BDT could be related to a dislocation core structure transformation in silicon.

Ab initio computations have been also conducted showing that those perfect dislocations in silicon have a stable configuration in the shuffle set [4] and that the mechanism, which can be involved in the core transformation into glide dissociated dislocations is associated to point defect migration [5]. However the properties of dislocation core structures have been found to be dependent on the nature of elemental semiconductors [4]. Indeed if in Ge the stability of such perfect shuffle core configuration has been confirmed, the calculations show that their mobility should be more important than in silicon. Contradictorily, in diamond it has been shown that such perfect shuffle dislocations are unstable and that the dislocations should be located in the glide set whatever the stress and temperature conditions. This last behaviour is due to the fact that diamond can accommodate sp² bonding into the core of dislocations. In these conditions the dislocation mechanisms at the BDT should be different depending on the nature of elemental semiconductors.

The aim of this paper is to compare the dislocation substructures obtained on elemental semiconductors below their usual BDT temperature. In this context single crystals of Ge, Si and diamond have been deformed below their usual BDT under a confining pressure of 5GPa [6]. The deformation microstructures have been characterized by TEM and will be discussed in relation with the results of the ab initio computations.

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Dislocation impurity interaction in Si

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Establishing knowledge on dislocation-impurity interaction is important from both the fundamental and practical viewpoints for development of semiconductor technology. Dislocation-oxygen interaction in Si is well known in terms of the dislocation immobilization due to preferential segregation and the findings are widely applied as basic knowledge in crystal growth and device fabrication processes. However, far less is known on the dynamic interactions of dislocation-impurity in Si heavily doped with electrically active impurities. This paper reports on the dislocation-impurity interaction in Si doped with various impurities at concentrations up to $2.5 \times 10^{20} \text{ cm}^{-3}$.

Dislocation generation was effectively suppressed in B-, P-, and As-doped Si when the concentration was higher than 10^{19} cm^{-3} . Dislocations were immobilized due to the impurity segregation and stable complex formation. B and N impurities promptly form strong locking agents, while P and As impurities form highly dense locking agents along dislocations. Dislocation velocity in Si doped with electrically active impurities increased with increasing concentrations of not only the donor (P, As, Sb) but also the acceptor (B) impurities in the temperature range of 650–950°C. N and Ge impurities had no or a little effect on the velocity of dislocations in motion. The velocity enhancement is attributed to the electrical effect of donor or acceptor impurities through the formation and/or migration of kinks as an elementary process of dislocation motion. It is remarkable that co-doping of Ge and B impurity is remarkably effective for immobilizing dislocations and retarding their velocity in Si.

Interface and Surface Controlled Plasticity in Nanostructured Metals

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The interactions of dislocations with internal interfaces govern the strength, strain-rate sensitivity and ductility of many nanostructured metals (PNAS 104, 3031; PNAS 104, 11155). Similarly, surface dislocation nucleation may govern the mechanical behavior of small-volume materials such as nanowires and nanopillars (Phys. Rev. Lett. 100, 025502). One can perform atomistic calculations to gain crucial information regarding dislocation-interface interaction processes, such as the activation volume of dislocation absorption, desorption and transmission at interfaces, and interfacial hardening response. With appropriate kinetic equations, such unit-process information can be employed to predict the strength and strain-rate sensitivity of nanostructured metals, that can be compared directly with experiments performed at seconds-and-minutes timescales.

Dislocation dynamics and the plasticity of single crystals

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Due to its complexity, the plasticity of single crystals is a benchmark tests for the further investigation of polycrystals and engineering materials. We present a few salient features of a predictive model for the plasticity of f.c.c. crystals in uniaxial deformation, which derives from an expanded form of the storage-recovery framework. In particular, it is shown by dislocation dynamics simulations that such continuum modeling is consistent with the coarse-grained properties of intermittent deformation by dislocation avalanches at a fine scale. The emphasis is on particular aspects of the well-known deformation stages that can now be explained in terms of individual or collective dislocation properties. This includes in particular the transition between dislocation stages, the orientation dependence of strain hardening and of the onset of dynamic recovery and the influence of multijunctions of strain hardening. Preliminary results on non-uniaxial deformation tests and the ability of this model to capture size effects in single and polycrystals will be discussed.

Preference: Oral presentation

Presenter: Ladislav Kubin

Rigorous homogenization results for dislocation dynamics

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We present some mathematical homogenization results of dislocation dynamics. More precisely, in the case of a single slip system, we consider a family of dislocation curves in a medium with periodic obstacles to the motion of these dislocations. In the special case where all the dislocations are contained in the same slip plane, we show that it is possible to get rigorously an effective macroscopic model. This macroscopic model is characterized by a nonlinear plastic law, which appears to be a byproduct of the homogenization procedure. We give in particular a method to compute numerically this plastic law, and we present some numerical results. In the special case of parallel straight dislocation lines interacting themselves and moving in a periodic potential, the model that we consider can be seen as a model of particles moving in interactions. Already in this case, our homogenization result seems new. In this framework and at a macroscopic level, we recover in particular the critical stress field associated to the pile-up of dislocations. We also exhibit a collective behaviour of dislocations.

Preference : Oral presentation

Modelling slip transfer across a tilt grain boundary in 2D discrete dislocation plasticity

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We present an approach to treat the transmission of edge dislocations across tilt grain boundaries in the framework of two-dimensional discrete dislocation plasticity. The key ingredient is a dynamically allocated source for the outgoing dislocation once an incoming dislocation hits a grain boundary and the orientation mismatch allows for transmission. Transmission occurs when the resolved shear stress on this source exceeds its strength and emits a dipole. One part of this dipole resides at the grain boundary and, together with the incoming dislocation, defines the residual Burgers vector, the other part is the transmitted dislocation. Values for the strength of this transmission source are obtained from atomistic simulations.

The approach is illustrated in the simulation of freestanding films in tension. Sizes are varied from near-bulk behaviour down to thin films with only one or a few grains across the thickness. The results for yield strength and hardening are compared with previous computations [1, 2] which assumed impenetrable grain boundaries.

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Atomistically-informed Dislocation Dynamics Simulations of Dislocation-Defect Interactions in fcc Crystals

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Perlado²

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When subject to irradiation or quenching, fcc metals with low stacking-fault energies are known to develop a microstructure characterized by a large number density of small stacking-fault tetrahedra (SFTs). Upon deformation, these materials undergo a very heterogeneous plastic behavior, with most of the strain localized along a few shear bands wherein SFTs are removed. The mechanisms of SFT removal by dislocations presumably govern the width and spatial distribution of these shear bands, and considerable effort has been devoted to their study by computer simulation. Although atomistic simulations have revealed numerous useful insights about these processes, they are too intensive to explore the full parameter space (dislocation character and length, SFT size, reaction geometry, etc) indeed present in real systems. In this work, we perform dislocation dynamics (DD) simulations of dislocation-SFT interactions for a wide range of conditions and SFT sizes. Our DD methodology is fitted from data obtained by specifically-tailored atomistic simulations. We provide strength curves as a function of the distance from the base of the dislocation glide plane, and identify the different mechanisms operating within each regime. We show that the strength of SFTs to dislocation passage can be universally described with a simple power law that depends only on the SFT area intersected by the dislocation glide plane.

Preference: Oral presentation

Presenter: Jaime Marian

The effect of the α - γ phase transition on dislocations in ferromagnetic bcc iron

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Body-centred cubic (bcc) iron develops an elastic instability, driven by spin fluctuations, near the α - γ phase transition temperature $T_c=912^\circ\text{C}$, which is associated with the dramatic reduction of the shear stiffness constant $c'=(c_{11}-c_{12})/2$ near T_c . Furthermore, at room temperatures and above, bcc iron is characterised by strong elastic anisotropy and thus the evaluation of accurate self-energies of dislocations in α -iron requires the use of the full anisotropic elasticity approximation. We show [1] that the elastic self-energies of straight edge dislocations strongly depend on temperature, and that the energies of both the 100 [001] and the 111[11-2] edge dislocations decrease sharply as we approach the temperature of the α - γ phase transition. The elastic self-energy of the 111[1-10] edge dislocations, on the other hand, remains almost independent of temperature up to the point of the α - γ transition. Using atomistic simulations and experimental information, we evaluate the core energies of dislocations, and show that the difference between the anisotropic elastic free energies of dislocations provides the fundamental explanation for the observed dominant occurrence of the $a\langle 100 \rangle$, as opposed to the $a/2\langle 111 \rangle$, Burgers vector configurations of prismatic dislocation loops in iron and iron-based alloys at elevated temperatures.

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Subgrains observed by high energy x-ray diffraction during in-situ loading

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By means of high angular resolution three-dimensional X-ray diffraction, individual subgrains are identified within a single grain in the bulk of a polycrystalline, macroscopic specimen. The broadened Bragg reflections consists of individual sharp peaks superimposed on a broad cloud of enhanced intensity. The sharpness of the peaks in all directions of reciprocal space and their integrated intensity allows their identification with almost dislocation-free subgrains.

These subgrains experience quite different backward elastic strains and cause distinct sharp profiles at different radial positions. Hence, the traditional composite model explaining the asymmetry of radial x-ray diffraction profiles by a superposition of two subprofiles corresponding to dislocation-rich dislocation walls and dislocation depleted cell interiors each broadened by their respective density must be modified and a statistical refinement of the composite model is presented.

Additionally, the evolution of the dislocation structure can be monitored during in-situ loading: Intermittent subgrain dynamics is observed during in-situ tension with individual subgrains emerging and disappearing in the course of deformation, indicating a rather volatile dislocation structure. During stress relaxation or unloading, significant changes are observed in the subgrain structure; the individual subgrains survive, but redistribute their internal stresses.

Invited presentation

Algorithm for Activated State Trajectory

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We describe the mapping of a recent algorithm for computing system activation trajectory in supercooled liquids onto activated state kinetics of dislocation mobility. The basis for exploring this isomorphism is that the new algorithm is autonomous, adaptive, and capable of uncovering mechanistic details of transition state processes. Moreover, it is relatively straightforward to implement, and has proved to be useful in probing potential energy landscapes in a different manner from the study of saddle points by Hessian diagonalization. Discussions will include speculative ideas on viewing creep phenomena as rheological response of matter to shear.

Interfaces within Discrete Dislocation Dynamics Simulations

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Abstract

Since the mid 80s [E.C. Aifantis, Trans. ASME, J. Eng. Mater. Technol. 106, 326, 1984] various gradient plasticity models have been developed for obtaining the plastic response of materials at the micron- and submicron- scales. It was not, however, until recently [e.g. K.E. Aifantis and J.R. Willis, J. Mech. Phys. Solids 53 (2005) 1047–1070] that interfaces were explicitly accounted for within a gradient plasticity formulation, according to which a separate interface energy term was attributed to all internal surfaces. Interfaces were, hence, allowed to follow their own yield behavior and an interfacial yield stress criterion was developed which predicted the stress at which dislocation transmission/emission could take place at an interface. Although experimental verification exists through nanoindentation, there remain unresolved issues concerning the physical interpretation of the internal length and interface energy terms involved in the theoretical formulation. Since the theory is based on the concept of dislocation pileups, discrete dislocation dynamics (DDD) simulations are performed on a tri-crystal with stiff and deforming grain boundaries in order to obtain a better physical insight towards these key material parameters. The strain distribution within the crystal obtained from the DDD simulations is in very well agreement with the analytical prediction derived from the gradient plasticity formulation. In particular it is noted that the internal length is equal to the dislocation source distance (order of μm), which was anticipated from the previous nanoindentation experiments.

A Generalized Peierls-Nabarro Model for Curved Dislocations

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Weinan E

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The Peierls-Nabarro model is a continuum framework incorporating atomic features for dislocations (line defects) in crystals. We present a generalized Peierls-Nabarro model for the core structure and dynamics of curved dislocations, in which the anisotropic elastic energy is obtained efficiently using the Fast Fourier Transform method, and the generalized stacking fault energy is used for the interplanar potential across the slip plane. Simulation results will be reported on dislocation core structures and activation energies of dislocation loops and kinked dislocations in Al, Cu and Si.

Non-singular Dislocation Fields

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Abstract

A simple but robust gradient elasticity theory is able to eliminate the classical elastic singularities in dislocation fields. The new solutions are simple and convenient to incorporate in revisiting classical dislocation-related problems. Some old but critical questions on dislocation cores, energies, interactions, and image forces, as well as grain boundaries and patterning are re-addressed along with some new questions on dislocation behavior under confinement (nanovolumes).

Viscoplasticity and plastic heterogeneities in ice single crystals loaded in torsion: a comparison between experiments and discrete dislocation dynamics simulations

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Abstract

Viscoplastic behaviour of ice single crystals is strongly anisotropic since plasticity essentially propagates by glide of dislocations in basal planes. In this paper, creep torsion tests are carried out on cylindrical ice single crystals machined so that the torsion axis matches with the crystallographic c axis. This induces shear stresses in the basal systems pushing basal screw dislocations toward the symmetry axis and no macroscopical force can drive the dislocations along any non-basal direction. Therefore, when confined to basal systems, dislocation glide can never explain the plastic flow experimentally observed. In this presentation we propose to invoke dislocation multiplication through cross-slip on prismatic systems to justify ice viscoplasticity. The scenario is tested using discrete dislocation dynamics simulations. Local rules are introduced in the dislocation dynamics code in order to mimic the probability for a basal screw dislocation to cross-slip on a prismatic system. A simulation campaign is then performed with different values of the applied stress. This leads to a creep law in which the shear strain rate is related to the square of the applied stress in good agreement with the experiments.

Statistical analysis of the plastic strain rate shows that the signal is scale invariant with the time. This is also the case for the experiments.

Finally, plastic strain heterogeneities are computed within the simulated volume and compared with X-Rays analysis. A statistical analysis shows that in both cases the distribution of the plastic strain amplitude is scale invariant. Moreover, it is found that the events are all correlated which denotes long-range interactions.

Preference: Oral presentation

Presenter: Marc FIVEL

Discrete Dislocation Plasticity Modeling of Polycrystal Plasticity

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Discrete dislocation plasticity analyses have mainly focused on the deformation behavior of single crystals. What has been less explored are the implications of the discreteness of dislocations for the mechanical response polycrystals. In this talk, a variety of discrete dislocation plasticity analyses of polycrystals will be discussed. The issues considered include: (i) the effect of grain boundaries on size effects in thin films; (ii) the transition from a single crystal sector crack tip field to a polycrystal HRR field; and (iii) the scaling in indentation with indentation depth and grain size. Although the analyses are limited to two dimensional plane strain conditions, the behaviors obtained are qualitatively, and sometimes quantitatively, in accord with experimental observations. In the analyses, grain boundaries are modeled as being impenetrable to dislocations. The implications and limitations of this assumption will be discussed.

Preference: Oral presentation.

Presenter Alan Needleman.

Migration of intergranular boundaries as a response of dislocation arrays to applied stress

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The intergranular boundaries with small misorientation angles are known to consist of periodic arrangements of dislocations. The simplest type is symmetrical tilt boundaries which are composed of only one set of dislocations. The motion of these dislocations perpendicular to the boundary plane will concurrently displace the boundary. However, by definition, dislocation motion is also associated with a shear deformation. Therefore, the motion of a small angle grain boundary must cause a shear deformation and hence, a shape change of the material.

Dislocations move and produce a shear when subjected to a shear stress. In the current study the mechanically induced migration of planar $\langle 100 \rangle$ tilt grain boundaries in aluminium bicrystals was experimentally measured. The results reveal that not only small angle, but also large angle boundaries with misorientation angles in the entire misorientation range between 0° and 90° can be moved by applied shear stress. Normal boundary migration was observed to be ideally coupled to a shear of the crystal region swept by the boundary. Boundaries with misorientations θ from opposite sides of the misorientation range ($\theta < 30^\circ$ and $\theta > 60^\circ$) move in opposite directions under an equally applied external stress. The measured ratios of the normal boundary motion to the lateral displacement of grains are in an excellent agreement with the corresponding boundary geometry and comply perfectly with the respective dislocation mechanics. From the measured temperature dependence of boundary mobility the migration activation parameters for different investigated boundaries were calculated. The mechanism of stress driven boundary motion coupled to a shear strain will be discussed.

Preference: Oral presentation

Presenter: Dmitri A. Molodov

ULTRASOUND AS A PROBE OF PLASTICITY? THE INTERACTION OF ELASTIC WAVES WITH DISLOCATIONS

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An overview of recent work on the interaction of elastic waves with dislocations is given. The perspective is to develop non-intrusive tools to probe plastic behaviour in materials. Ideas and methods are first worked out in two dimensions for simplicity, and results in three dimensions are then described. They explain a number of recent experimental findings, including the frequency dependence (quadratic and quartic) of ultrasound attenuation in copper, the visualization of the scattering of surface elastic waves by isolated dislocations in LiNbO_3 , and the ratio of longitudinal to transverse wave attenuation in a number of materials.

Specific results reviewed include the scattering amplitude for a bulk elastic wave by a single pinned dislocation segment in an infinite elastic medium, and the surface wave scattering by a single sub surface dislocation in a semi infinite medium. Also, using a multiple scattering formalism, expressions are given for the attenuation coefficient and the effective speed for the coherent propagation of elastic waves in a three dimensional medium filled with randomly placed and oriented dislocation line segments, also with randomly oriented Burgers vectors. The usual Granato-Lücke theory is a special case of the developed formalism.

Preference: Oral presentation

Presenter: Fernando Lund

Perfect dislocations mobility in silicon: theoretical study of kinks formation and migration

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Silicon, usually considered as a prototype for zinc-blende covalent materials, has been extensively studied, and most of its properties are well known. For instance, we have now a good understanding of high temperature plasticity, key dislocations being Shockley partials, moving by formation and migration of kink pairs. At low temperature, although silicon is brittle, scratch tests and deformation experiments under high confining pressure have revealed the presence of perfect undissociated dislocations, with several orientations. However, we know very little about the mobility of these dislocations, and in particular about the possible role of thermally activated mechanisms such as kinks formation and migration, like for partial dislocations.

Using first principles and interatomic potentials calculations, together with the Nudged Elastic Band method, we have investigated properties of kinks on a non-dissociated screw dislocation in silicon. Atomistic mechanisms allowing formation and migration of these kinks, as well as associated activation energies, have been determined. Contrary to partial dislocations at high temperature, we found that the kinks are highly mobile, even at low temperature, but that a large energy is required for their formation. The effect of stress on these mechanisms has also been studied, and has to be considered to explain the mobility of perfect dislocations at low temperature. Finally, we discuss our results in relation with experiments, and show that it seems unlikely that the observed transition between partial and perfect dislocations could be solely attributed to stress.

Preference: Oral presentation

Presenter: Laurent Pizzagalli

Dislocation Patterning and Formation of Omega Phase in Shock-Loaded Tantalum

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In this talk, we will present the results obtaining from transmission electron microscopy studies of shock-loaded tantalum, a group V transition metal that exhibits no clear solid-state phase transformation under static-pressure conditions, to evidence and verify the occurrence of shock-induced phase transformation under peak pressures above 30 GPa. Since the domains of omega phase are frequently found in regions containing high-density lattice dislocations with no cell-wall formation, we suggest that the shock-induced phase transformation in tantalum is heterogeneously nucleated through the catalysis of lattice dislocations with a unique patterning configuration when the dynamic recovery process for cell-wall formation becomes largely suppressed under dynamic pressure conditions. A path (strain-rate) dependent dislocation mechanism based upon the heterogeneous clustering of closely spaced dislocation loops generated from a jogged screw dislocation is proposed to rationalize the shock-induced phase transformation in tantalum.

Preference: Oral presentation

Presenter: Luke Hsiung

Origin of Dynamic Strain Aging in Metals: Solute Aging of both Mobile and Forest Dislocations

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Abstract

A full rate-dependent constitutive theory for dynamic strain aging is developed based on two key ideas. The first idea is that both solute strengthening and forest strengthening must exist and must exhibit aging phenomena. A full rate theory clearly shows that neither alone can yield negative strain-rate-sensitivity under normal assumptions. The second idea is that a single physical aging mechanism, cross-core diffusion within a dislocation core, controls the aging of both the solute and forest strengthening mechanisms. All of the material parameters in the model, aside from forest dislocation density evolution parameters, are derivable from atomistic-scale studies so that the theory contains essentially no adjustable parameters. In application to a variety of Al-Mg alloys, the model predicts the steady-state stress/strain/strain-rate/temperature/concentration dependent material response, including negative strain rate sensitivity, in qualitative and quantitative agreement with available experiments. With no additional assumptions, the model also reveals the origin of non-additivity of solute and forest strengthening and explains the observed transient stress behavior in strain-rate jump tests. The theory thus captures essentially all aspects of the dynamic aging phenomenon.

Stress Functions for Dislocation Loops in Anisotropic Crystals

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Stress functions have been used to calculate material properties associated with elasticity. For example, the second derivatives of Airy's stress function correspond to stress components in plane strain problem. For the case of dislocations, stress function has been so far applied to computational simulations etc. The stress functions used in the simulations were usually derived on the basis of isotropic elasticity theory. However, almost all crystals belong to anisotropic elastic body in the continuum elastic limit. Therefore, it is very important to take into account the anisotropy to study dislocations in actual materials. In order to stimulate investigations in terms of the anisotropic elasticity theory, we obtain explicit expressions of stress functions for dislocation loops in anisotropic crystals. As a result, interaction energy of dislocation loops can be estimated by double line integral along the dislocation lines.

Grand Scaling of the Temperature Dependence of the Strength of Crystals Governed By the Peierls Mechanism

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The temperature dependences of the critical resolved shear stress (CRSS), governed by the Peierls mechanism, of $\{110\}\langle 110\rangle$ and $\{001\}\langle 110\rangle$ slips in pure NaCl type crystals, those of $\{111\}$ slip in pure bcc transition metals, those of $\{111\}\langle 110\rangle$ slip by the dissociated dislocation in covalent crystals of the diamond and the zinc blende structures and those of $\{111\}\langle 110\rangle$ slip by the perfect dislocation at low temperatures in zinc blende crystals have been demonstrated to be well scaled for each slip with respect to the non-dimensional normalization of the CRSS by the shear modulus G and the temperature by Gb^3/k_B , where b is the strength of the Burgers vector and k_B the Boltzmann constant. These normalized CRSS vs. T relations for five types of slip have been shown to be further rescaled universally by renormalizing CRSS by the estimated Peierls stress $\tilde{\sigma}_p$ and the temperature by the kink pair energy parameter of $(\tilde{\sigma}_p/G)^{1/2}(bd)^{3/2}G/k_B$, where d is the period of the Peierls potential. The success of this grand scaling of the temperature dependence of the strength indicates that the low temperature strength of crystals governed by the Peierls potential can be estimated from the measurement of the CRSS at high temperatures.

Preference: Oral presentation

Presenter: S. Takeuchi

3D-Continuum Theory of Dislocations: Numerical Implementation and Application

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Key Words: *continuum theory of dislocations, crystal plasticity, numerical implementation*

The growing demand for physically motivated continuum theories of plasticity led to an increased effort on continuum descriptions based on dislocations. For simplified systems of straight parallel edge dislocations in a single slip configuration a dislocation-based plasticity theory is available, which was rigorously derived with methods of statistical mechanics for interacting particle systems.

However, earlier attempts to transfer this method to three-dimensional systems of curved dislocations failed due to the inability of the classical dislocation density measures to reflect all dislocations as line like objects.

This deficiency was remedied by a recently introduced advanced continuum theory of dislocations (Hochrainer 2006). This theory utilizes a generalization of the dislocation density tensor, the so-called dislocation density tensor of second order, α^{II} . Within this tensor all dislocations are considered as line-like objects. Hence, the common distinction between geometrically necessary and statistically stored dislocations is dispensable in this framework.

We study the extended continuum theory for the quasi-2-dimensional case of a single glide system. We numerically validate this special case by showing that the continuum evolution equation of this new dislocation density measure can handle the kinematic evolution of discrete dislocations. The constituents of the evolution equations and the effect on the numerical implementation will be explored by numerical examples.

We show how impenetrable boundary conditions can be modeled within the advanced continuum theory. Dislocation pile-ups at impenetrable boundaries are studied and compared to the treatment by other dislocation density-based models.

By embedding the evolution equations (on the meso-scale) into a crystal plasticity context (on the macro-scale) we study the stress field evolution inside a plastic slip channel and for a composite material. The required steps are very generic and demonstrate the versatility of the extended continuum theory.

Preference: oral presentation

Presenter: Stefan Sandfeld

Energy flow around a moving dislocation

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When a dislocation moves in a lattice, it accelerates and decelerates according to the periodic Peierls potential and emits lattice waves. Although they affect the velocity of the dislocation, the strength of the emitted waves and the energy flow around the moving dislocation are not clear. In this paper, we make a molecular dynamics simulation of a dislocation moving in a simple lattice to clarify these problems.

The crystal is a simple cubic lattice. Each atomic row directed parallel to the z-axis moves rigidly only parallel to this direction. A straight screw dislocation is introduced and motion of all atomic rows is traced by integrating the equations of motion. The inter-atomic row potential is sinusoidal and acts between the nearest neighbor atomic rows. The energy flow is traced by calculating the work on each atomic row done by the nearest neighbor atomic rows.

When the applied stress is small and the dislocation in the unstable equilibrium position falls down to the nearest Peierls valley, the magnitude of the emitted energy is the difference of the potential energy in the core region between the two states. When the applied stress is large and long distance motion of the dislocation occurs, the energy flows towards the slip plane vertically from the surrounding atoms. The energy is concentrated into a sharp beam and is emitted behind the dislocation.

3-Dimensional Dislocation Dynamics Modelling of Hardening effects of Radiation Damage in Iron

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Abstract

3D dislocation dynamics simulations have been carried out to model the interaction between prismatic loops and dislocations in pure iron subject to uniaxial loading conditions. The program used was a modified version of the MicroMegas code developed by Devincre, Kubin et al. The primary goal of the simulations was to understand the mechanisms of interaction of $a/2 \langle 111 \rangle$ interstitial loops and a mobile dislocation. The secondary goal was to investigate the dependence of the critical stress needed for dislocations to overcome the obstacles as a function of size of loops and their orientation with respect to the glide plane. The simulations have shown various possible complicated 3D interactions in which in the mobile dislocation bows around a loop, either reacting with the loop dislocation or leaving it behind unchanged. The dependence of the critical stress on the size of the loops and the initial configuration will also be described and compared to results for molecular-dynamics simulations of similar interactions..

3D - Stress analysis during crack-crazing patterns interactions in a polystyrene material

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Abstract

In this study, interactions between a main crack and a surrounding layer of crazing patterns in a polystyrene material (PS) are considered. A stress field distribution induced during these interactions is based on the resolution of some differential equations along with appropriate boundary conditions and the use of a numerical approach. These equations are established according to Mohr's criteria since the craze growth occurs along directions parallel to the minor principal stress axis. Because this damage can constitute an important toughening mechanism, the mode I Stress Intensity Factor (SIF) is employed to quantify the effects on a crack of the damage consisting of crazing patterns. It is proven, herein, that crazes closer to the main crack dominate the resulting interaction effect and reflect an anti-shielding of the damage while a reduction constitutes a material toughness.

Keywords: Displacement, stress, strength, major and minor principal stress, crack, crazing patterns.

Stress analysis during the interaction between dislocations and a main crack: Case of a bi-material

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The stress and displacement fields of an edge dislocation near a semi-infinite or a finite interfacial crack are formulated using the complex potential theory of Muskhelishvili's elasticity treatment of plane strain problems. It is known that the image forces exerted on the dislocation have an oscillatory character with respect to the dislocation position if the dislocation is originated elsewhere and moves to the vicinity of a finite interfacial crack. It is proven herein that there is no such oscillation of image forces if the edge dislocation is emitted from the finite interfacial crack or if the crack is semi-infinite. Thus, the Stress Intensity Factor (SIF) in the case of an edge dislocation produces an oscillatory character for both semi-infinite and finite interfacial cracks. In this study, it is shown that the SIF depend on whether the dislocation is emitted from the crack or comes from elsewhere.

Keywords: Displacement, strain, stress, dislocation, image forces, stress intensity factor.

Breakdown of Self-Similar Hardening Behavior in Au Nanopillar Microplasticity

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In this work we study of scale effects in Au nanopillars under compression. We propose that plastic yielding in these nanostructures is characterized by a critical lengthscale at which a transition from volumetric to surface dominated plasticity takes place. This transition effectively sets a lower-bound on the self-similar behavior commonly assumed in nanostrength models. Using Quasicontinuum simulations we study the subcritical regime and find that plasticity at these scales is governed by dislocation emission at surface irregularities.

Preference: Oral presentation

Presenter: Jaime Marian

New in situ experiments in Fe at low temperature

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Atomistic calculations have renewed the interest for experimental studies of dislocation mobility in iron and iron alloys. Since the only available results of in situ experiments have been obtained in the 70's, more accurate and more quantitative data are needed, in order to determine the exact dislocation kinetics and slip planes, as a function of temperature and local stress. In particular, the discontinuities observed in the temperature dependence of stress, activation volume, and pre-exponential term, indicate a possible change of mechanism at around 200-250K.

New in situ experiments have been carried out in pure Fe, between 110K and 400K. The videos show that straight screw segments glide and cross-slip between $\{110\}$ planes, where they are subjected to a high frictional stress. Two different kinds of kinetics are observed as a function of temperature:

- In the higher temperature range, close to room temperature, screw dislocations segments move steadily, as expected from a kink-pair mechanism. The close inspection of dislocation sources shows that they move at a velocity proportional to their length, in agreement with the corresponding model.
- In the lower temperature range, screw dislocations move jerkily. They remain locked in a Peierls valley during several seconds, then jump in a $\{110\}$ plane over several tens of nanometers during less than 1/50 s, till they are locked again, and so on.

The jerky motion at low temperature is similar to that already observed in prismatic planes of h.c.p. metals, and in several intermetallics. It is inconsistent with a kink-pair mechanism, for which the motion between adjacent Peierls valleys yields a smooth motion with almost constant instantaneous velocity. It corresponds instead to a "locking-unlocking" mechanism, for which dislocations are able to glide freely over several hundreds of interatomic distances between sessile positions in Peierls valleys. Such a free motion requires the existence of a metastable-glissile core configuration, with very short life-time under stress. The modelling of the transition between kink-pair and locking-unlocking mechanisms, in the elastic approximation, shows that it can account for the discontinuity of the plastic properties observed at 200-250K.

Nanoindentation studies of Dislocation-Grain Boundary Interactions

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We have been using nano-indentation to study the relative strength of grain boundaries as barriers to slip. The localised deformation around a nano-indent allows individual grain boundaries to be selected and analysed.

In Fe-0.01wt% C (bcc) polycrystals we have found very marked 'pop-ins' associated with indents near grain boundaries. These pop-ins are typified by a distinct increase in hardness prior to a marked displacement excursion at near constant load, followed by a drop in hardness to levels seen for indents remote from the grain boundary. These pop-ins occur at much greater depth than pop-ins associated with the initial nucleation of dislocation loops during the early stages of indentation, and for a given boundary the pop-in occurs at lower load and indent depth when the indenter is closer to the boundary. The pop-ins allow the resistance to slip transfer to be studied as a function of the grain boundary geometry. Resistance to slip transfer increased with misalignment m of slip system across the grain boundary. With m given by the product of cosines of the angles between the best aligned slip directions and slip planes in the two grains.

Despite extensive testing the grain boundary associated pop-ins were not observed in the following systems Cu (fcc), interstitial free steel (ferrite (bcc) with 0.002wt% C), Fe-0.01wt% C (bcc) immediately after prior plastic deformation. This indicates that the pop-in is associated with the activation of dislocation structures pinned by C (and other interstitials) either in the boundary itself or close to the boundary within the neighbouring grain. Hardening is caused by the build up of large dislocation pile-ups at the grain boundary, which then suddenly release resulting in the excursion, slip transfer is subsequently significantly easier and so the hardness drops. In the absence of interstitial pinning slip transfer is markedly easier so that large dislocation pile-ups are generated at the grain boundary and consequently the large pop-ins are not seen.

Investigation of dislocation mobility in small periodic cells using the Nudged Elastic Band method: effect of a confinement pressure

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Dislocation Peierls stress is usually computed by applying an increasing shear strain on a system encompassing one or several dislocations. While such an easy approach is very efficient for large systems, it remains more difficult to use in combination with first-principles methods, for which small calculation cells are mandatory. Whether periodic or cluster-like boundary conditions are used, one has to take care of spurious contributions related to small systems sizes. We present here a new general approach, allowing to investigate the displacement of a dislocation into a crystalline lattice with no boundary effects, in periodic cells. All dislocations in the cell are coherently displaced together, by using the Nudged Elastic Band method. We applied this technique to study the displacement of a non-dissociated screw dislocation in several materials with a zinc-blende structure, modelled in a first-principles framework. Compared to usual methods, we have been able to obtain the dislocation structure and the associated energy variation during the displacement, even for non easy directions. The effect of a confining pressure has also been determined, showing that it may significantly increases or decreases the dislocation mobility according to the selected direction.

Preference: Oral presentation

Presenter: Laurent Pizzagalli

Atomistic calculations of the formation, stability and mobility of a non dissociated 60° dislocation in silicon

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There have been very few investigations related to the non-dissociated 60° dislocation in zinc-blende materials. The main reason is that it dissociates in two Shockley partials at high temperature, in the usual experimental conditions, in the ductile domain. Also, at low temperatures, although non-dissociated dislocations have been shown to exist, most studies have focussed on the screw dislocation, since it is expected to govern the plasticity. Nevertheless, recent theoretical investigations have shown that a large stress applied to a surface step could lead to the formation and propagation of a perfect 60° dislocation in silicon, at low temperature, growing the need for a better characterization of this defect.

We present here the results of atomistic simulations, performed with first principles, tight-binding and interatomic potential calculations, of the formation, stability and mobility of a non-dissociated 60° dislocation in silicon. First, it is shown that while a glide core is much more stable than a shuffle core, only the latter can move under the effect of an applied stress. The mechanism underlying dislocation mobility is analyzed. Regarding nucleation, we show that a shuffle 60° dislocation can form at a surface step, but also in the vicinity of a crack front, suggesting that this defect could have a major influence on the mechanical behavior of covalent materials.

Preference: Poster presentation

Presenter: Laurent Pizzagalli

Matching asymptotic expansion in modelling of edge dislocation pile-ups

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The approach suggested in [1, 2] is developed further to derive the equilibrium distribution of n edge dislocations in a linear pile-up stressed by a constant applied loading against an interface in a bimetallic solid. As $n \rightarrow \infty$, the dislocation positions are located with sufficient accuracy that the stress distribution at the interface can be evaluated by a simple computational procedure. The stress is found as a prefactor of the singular part, which is mathematically analogous to a "stress intensity factor" in continuum fracture mechanics. The stress is determined to high accuracy from a lumped discretization of superdislocations away from the interface. We present an example in which a hundred dislocations can be replaced by just four superdislocations with only a 1 per cent error in the computation of the stress at the interface. Then a discussion is given of how the structure of the pile-up depends on the materials parameters.

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Preference: Oral presentation

Presenter: R.E. Vaskoboinikov

Evaluation of recovery kinetics of AA3103 using stress relaxation tests

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Abstract

Recovery processes are based on rearrangement and annihilation of dislocations by climb and cross-slip. They are of significant scientific and technological relevance especially for materials with high stacking fault energy, e.g. aluminum alloys. However, over the years less scientific interest was drawn to this softening process. Even though physics based flow stress models are relied on the evolution of dislocation density especially at elevated temperatures. Hence there is a need to advance our understanding of recovery in particular with regard to through-process modeling.

Within the scope of the project stress relaxation and double tension tests at elevated temperatures were performed on a commercial aluminum alloy 3103. The recorded stress-time evolution based on stress relaxation and double tension tests were compared to gain a better understanding of the mechanisms governing the recovery processes and to obtain a reliable evaluation of the recovery kinetics as well. The evaluation of recovery kinetics by means of stress relaxation tests provides important complementary information to standard annealing tests. In addition the effect of an applied load on recovery processes can be studied. The recovery behavior with and without load will be discussed. Finally, the obtained information will be utilized for a through-process modeling exercise.

Preference: Poster

Presenter: Sheila Bhaumik

Peierls-Nabarro model and kink pair nucleation in MgO

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Considerable heat and mass transport take place in the Earth's mantle. These processes are responsible for plate tectonics and related phenomena such as volcanism or earthquakes. The study of the plastic properties of rocks and minerals is thus of primary importance to model the rheology of the mantle. Magnesio-wustite (Mg,Fe)O is one of the main constituents of the lower mantle (between 670 and 2900 km depth). Unfortunately, deformation experiments on MgO under the extreme P, T conditions relevant of the Earth's lower mantle are still very delicate. Numerical simulations provide an alternative to address the behaviour of materials under extreme conditions. In this study, we present calculations of dislocations properties under extreme pressure (up to 100 GPa).

Dislocations core calculations are performed within the framework of the Peierls-Nabarro (PN) model for three relevant slip systems of the rock salt structure, $\frac{1}{2}\langle 110 \rangle \{110\}$, $\frac{1}{2}\langle 110 \rangle \{001\}$ and $\frac{1}{2}\langle 110 \rangle \{111\}$. *Ab initio* calculations of Generalised Stacking Fault (GSF) were determined for various pressure ranging from 0 to 100 GPa. Results of GSF calculations are then used as input of PN model to determine dislocations core spreading and Peierls potentials. Finally, activation energies of rectangular kink pair are calculated using the Peierls potentials previously determined.

We found that, as expected, MgO deformation is dominated at low pressure by $\frac{1}{2}\langle 110 \rangle$ slip in $\{110\}$. Whatever the pressure, our results show that activation energy of kink pair nucleation decrease with applying stress. At low pressure, we are able to reproduce in some extend the evolution of critical resolved shear stress as a function of temperature. Finally, when increasing the pressure up to pressure relevant to the Earth mantle, we found that the plasticity of MgO may be governed by $\frac{1}{2}\langle 110 \rangle \{001\}$ slip systems.

Preference: Poster presentation

Presenter: Philippe Carrez

Dislocation modeling of perovskites using the Peierls-Nabarro model

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MgSiO₃ perovskite is the most abundant phase of the lower mantle and accounts for half of the Earth's mass whereas in the lower mantle (i.e. at depths between 670 and 2900 km), calcium is hosted by another perovskite structure: CaSiO₃. We have used the Peierls-Nabarro model (incorporating *ab initio* calculations of generalized stacking faults) to calculate dislocation properties of three perovskite structured materials: SrTiO₃, CaSiO₃ and MgSiO₃. Cubic SrTiO₃ is a structural analog of CaSiO₃ and allows numerical models to be compared with experimental data (deformation experiments (Brunner *et al.* 2001), high resolution TEM (Jia *et al.* 2005) electronic structure (Zhang *et al.* 2002)). Dislocation core profiles have been calculated in CaSiO₃ perovskite at 0, 30 and 100 GPa (the pressure in the lower mantle ranges from 25 to 130 GPa). At 30 GPa, <100>{1-10} exhibits negligible lattice friction, an unusual characteristics for a silicate. This slip systems hardens however at 100 GPa. In MgSiO₃ perovskite, SiO₆ octahedra are tilted resulting in a lowering of the symmetry from cubic to orthorhombic. The orthorhombic distortions are found to have a strong effect on lattice friction.

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Mechanical behaviour and deformation mechanism of a niobium alloy with different carbon content

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Nb-based alloys are one of the most promising refractory metals for use at high temperatures, because, although these alloys need to be coated, Nb has a high melting point of 2741K and a relatively low density, as well as advantages in respect of alloying and manufacturing. The strength of Nb decreases substantially at temperatures above 1000K but may be improved by various approaches, including solid solution strengthening, and dispersion or composite strengthening with intermetallic compounds, as well as with carbide.

As a potential structural material designed for service at elevated temperature, strength, creep resistance and microstructural stability are very important. This study, therefore, evaluates the mechanical behaviour, carbide coarsening rate and deformation mechanisms of Nb-Ti-Al alloys with different C contents. The results show that: the presence of extensive carbides led to a substantial increase in yield strength at room and high temperatures and creep resistance but a dramatic decrease in toughness; at room temperature all three alloys deform primarily by slip, with mechanical twins; deformation at higher temperatures occurs by a combination of dislocation glide and climb processes, giving more homogeneous microstructures; most of the dislocations in the matrix of these alloys have Burgers vector $b=1/2\langle 111 \rangle$ although some short segments with $b=\langle 100 \rangle$ were also observed where two dislocations with $b=1/2\langle 111 \rangle$ interact during high temperature deformation; deformation of carbide at high temperatures occurs primarily by $\{111\}\langle 110 \rangle$ slip.

SOME CORRELATIONS BETWEEN SLIP BAND EMERGENCE AND DISLOCATION PATTERN

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The aim of present work is the study of various forms of the plastic deformation of single crystals of nickel alloys oriented for single slip [135] and multiple slip [001]. Particular attention is paid to the heterogeneity of deformation observed at two distinct scales: the slip bands and the dislocation organizations. The slip bands emerging at the surface can be studied using the atomic force microscopy (AFM) [1,2]. The height of extrusions and inter-band spacing depend on the orientation of tensile axis, the strain level and the nature of the alloy. At another scale, dislocation organizations typical of f.c.c. crystal have been observed which depend on the orientation of tensile axis and on the stacking fault energy [3]: long cells with crystallographic walls (near (111), type I), equiaxed cells (type II) and long cells with non-crystallographic boundaries (type III). A study by transmission electronic microscopy (TEM) has enabled us to approach the dimensional characteristics of these structures. In the case of mono-crystal oriented for single slip straining in stage III ($\gamma \approx 0.7$) we observed a correlation between the inter-band spacing (d) and the inter-wall spacing (λ) of the type I dislocation pattern. This result suggests that this kind of walls is a barrier to the mobility of dislocations unlike equiaxed cells that would be only an obstacle to the dislocation mobility. This internal length is about 3 μm for nickel and 500 nm for Ni16%Cr alloy. Consequently, stacking fault energy is probably a parameter which affects the internal length in relation with cross-slip capability. On the other hand, the [001] direction, enabling multiple slip, lead to more complex results in the nickel. Indeed, only equiaxed cells are observed for this orientation with cell sizes (λ) in the order of 427 nm and 600 nm for respectively shear strain (γ) of 0.5 and 0.8. These magnitudes are far lower than those observed for inter-band spacing ($d \approx 1.4 \mu\text{m}$). As in the case of samples oriented for single-slip, the equiaxed cells observed for samples oriented for multiple-slip seem to be only as obstacles to the mobility of dislocations. By contrast, there are probably walls associated with this kind of cells which act as barriers to the movement of dislocations. These are hardly discernible in TEM but their spacing can be identified by AFM. In particular, a study of the variance associated with inter-band spacing as a function of deformation should provided some new interpretation of the various hardening stages.

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Atomistic simulation of He bubble in Fe as obstacle to dislocation

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In the development of ferritic materials for fusion technology the studies in irradiation defects have become an essential subject because of their detrimental effects on the mechanical properties. In the nuclear fusion reactors high rate of insoluble helium are generated in metals due to transmutation reaction. There is thus a high tendency for helium atoms to meet each other and form nanometric bubbles. The effect of He bubbles on the mechanical properties is still unclear. In this work molecular dynamics (MD) simulation is used to investigate the state of the He bubble and its interaction with an edge dislocation in Fe as a function of the He content and temperature. Different interatomic potentials for Fe-He are used. Results show that the bubble expands with increasing He content and it may solidify at temperatures below 300 K due to the surrounding Fe crystal and high internal pressure. We observed that He bubble could be a soft or hard obstacle to the motion of the dislocation. We showed that the bubble size and temperature could strengthen and weaken the interaction, respectively. The creation of self-interstitial atoms due to loop punching and their interaction with the dislocation is the main strengthening mechanism at high He contents. Different strengthening levels are observed depending on the interatomic potential. Review of our results will be presented here.

Study of dislocation nucleation activation from surface step by atomistic calculations

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Contrary to bulk materials, in which plasticity is often linked to the presence of Frank-Read sources, nanostructured materials are too small for such sources to operate. Plasticity is then mainly due to the nucleation of dislocations from surfaces and interfaces. In free surfaces, irregularities such as steps are expected to be favored sites for the formation of dislocations. Nucleation, happening at small spatial and temporal scales, is difficult to observe experimentally. An alternative is atomistic simulations, allowing to investigate the very first stages of plasticity.

We present here an analysis of the dislocation nucleation activation from a surface step in a crystal under stress, studied by atomistic calculations. Two model materials are considered: a face centered cubic metal (aluminum) and a diamond-like semiconductor (silicon), both of them being modeled with semi-empirical potentials.

Finite temperature simulations in aluminum lead to the formation of dislocation half-loops, and allow the determination of saddle-point configurations and the associated activation energies. In order to investigate a wide range of applied stress, different methods have been used: molecular dynamics simulations, and nudged elastic band calculations. The obtained results are then compared with those deduced from elasticity.

In the case of silicon, the determination of the activation parameters is more complicated because of the numerous different types of dislocation that can be obtained, depending essentially on the temperature. Nevertheless, the simulations bring important information on a possible change of nucleation mechanisms with temperature, namely nucleation of perfect dislocations in the shuffle set at low temperatures and partial dislocations in the glide set at high temperatures.

Preference: Oral presentation

Presenter: P. Hirel

Incorporating Nonlinear Elasticity into a 2D Theory of Dislocations

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Starting from the equation of motion of individual dislocations, a continuum description of a 2D dislocation system was derived by Groma and his co-workers for single slip, which is, according to earlier investigations, able to predict dislocation and GND densities under many different boundary conditions. This theory and all other models proposed so far in the field are based on the assumption that the medium which contains the dislocations can be described by linear elasticity. Many authors speculated, however, that nonlinear effects may have an important role in PSB formation of dislocations during fatigue experiments. That would, for instance, make a difference between the energy of an interstitial and vacancy type dislocation dipole.

The goal of the investigations presented in this talk is to study how nonlinear behaviour of the medium affects the dislocation dynamics. In the equation of motion of a single dislocation an extra term, which contains the effect of the introduced “extra physics”, is derived analytically [1]. It is shown that the modified model, contrary to the linear case, has spatially periodical solutions, i.e., a dislocation pattern evolves from a homogeneous distribution. The length parameter of the pattern is about the average distance of the dislocations. We also analyse the results of numerical discrete dislocation dynamics simulations, when relaxations from different random initial states have been performed, and prove the appearance of the length parameter mentioned above.

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Preference: Oral presentation

Presenter: Péter Dusán Ispánovity

Dislocation Structure Evolution of Al alloy Deformed at a High Strain Rate

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In order to understand the development of the dislocation microstructure and its connection with the mechanical properties of the materials deformed at a high strain rate, electron microscopical studies have been conducted for Al alloy deformed by the split-hopkinson bar test and a tube compression process by electromagnetic forming (EMF) at high strain rate ($\sim 10^3/\text{s}$). The results of the split-Hopkinson bar test provided us with basic information on the mechanical behavior and dislocation structure evolution during a high strain rate deformation. An inhomogeneous deformation such as a buckling was observed by an electromagnetic tube compression process. The variation of the dislocation configurations produced by the electromagnetic tube compression was investigated by using the TEM weak beam dark field imaging technique. Nano indentation technique was used for a measurement of the mechanical properties of the inhomogeneous deformed region. Based on the experimental results, the correlation between a dislocation structure and the mechanical properties of an inhomogeneous deformed region by electromagnetic tube compression is discussed.

Plasticity of Miniaturized Tension and Compression Samples

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In the last five years, size effects exhibited by micro-compression specimens gained a lot of interest. While this method offers a possibility to investigate the plastic deformation of micro-crystals in the absence of strain gradients, there are several experimental drawbacks. There is a limited aspect ratio for these samples due to plastic buckling. Inhomogeneous stress and strain fields can arise due to taper of the specimens, leading to strain gradients over the specimen height. Furthermore, several geometrical constraints are present at the sample top and base. Therefore, a new micro-tensile testing method was developed to overcome these limitations. Focussed ion beam machining was applied to fabricate micro-tensile specimens and the sample loading was performed in-situ in a scanning electron microscope. Beside proper alignment, this enables to monitor the sample deformation and to correlate it to the measured mechanical data. We studied the influence of crystal orientation and aspect ratio on the deformation behaviour of single crystal copper specimens with critical dimensions between 0.5 μm and 8 μm . Furthermore, the influence of the loading mode on the observed size-dependent mechanical properties is discussed with respect to the evolving local microstructure investigated by Laue and electron backscatter techniques.

Deformation substructure formation

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Spontaneous structural inhomogeneity is the most distinguished mesoscopic feature of plastic deformation of ductile crystalline materials. The formation of a subrostructure is interpreted as an adjustment of the lattice space to minimize the work needed to obey imposed loading conditions. There are three basic mechanisms of work minimization: strain localization, local misorientations of the lattice space and building of generation-annihilation centers. The stain localization into shear and kink bands provides a favorable flow path in the case of strain softening. The misorientation causes fragmentation of the lattice space into structural elements with locally decreased number of active slip system and that way the misorientation avoids the energy costly multislip. The generation-annihilation centers on the one hand produce new glide dislocations maintaining their optimum density, on the other hand, they serve as sinks for dislocation debris generated during deformation. The minimum work principle is formulated in terms of virtual work for a deformed crystal subjected to boundary conditions and dissipation inequality. Having no length scale, the standard continuum theory predicts infinitesimally small structural size. Incorporating non-local effects caused by short-range correlations among dislocations the proposed model predicts misorientations of structural elements and their size.

Grain boundary sliding induced by lattice dislocation activity during ambient temperature creep in h.c.p. metals

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H.C.P. metals and alloys show significant creep behavior even below the 0.2% proof stress at ambient temperature, which is caused by straightly-aligned dislocation arrays of single slip system without any dislocation cuttings inside a grain. It results in weak work-hardening inside a grain, but pile-up of dislocations at grain boundary (GB), because of the violation of the von Mises law. To continue creep deformation, these piled-up dislocations have to be accommodated. In the present study, we performed EBSD analysis and AFM observation on Zn specimens after creep test at ambient temperature to infer the GB accommodation mechanism. The sample was Zn with several grain diameters (d) of 100, 210 and 1500 μm and the crept temperature was from 203 K to 473K. The creep results show grain size dependence, where increasing grain diameter restricts creep strain, different from high temperature creep. The sample with $d = 1500 \mu\text{m}$ fractured just after loading because of stress concentration at GBs. EBSD analyses revealed that the crystal lattice gradually inclines near GB, which mean dislocations pile up near GB. Therefore, grain boundary is accommodation site clearly. AFM observations showed 0.26 μm grain boundary steps, which reveal the evidence of grain boundary sliding. These observations disclose that grain boundary sliding was induced during ambient temperature creep as an accommodation. Another important result is that apparent activation energy of ambient temperature creep is 18 kJ/mol, which is one-third of that of grain boundary diffusion. It means atomic diffusion is difficult to be activated. Therefore during the creep, lattice dislocations were considered to be pushed into GB through shuffling, shorter atomic jump than lattice diffusion. This shuffling is activated with a low apparent activation energy, and is considered to control the creep deformation at ambient temperature.

Preference: Oral presentation

Presenter: Tetsuya Matsunaga

In-plane work hardening effect of dislocation loops in particle strengthened alloys

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A Frank-Read dislocation source is activated at a critical external applied stress that depends on its size. The newly created dislocation loop will expand under this stress if the latter suffices to overcome the stresses from obstacles like second phase particles, in addition to the loop's self stress. On the other hand, the loop causes a stress on the source that created it, such that to some degree, it shields the external stress acting on the source. Hence after a Frank-Read source has been activated by the quoted critical external stress once, it will not be activated again unless either the loop and its shielding effect vanish in grain boundaries or free surfaces, or if the external stress is increased further. When a second loop is created, the source will be shielded even more, and so on. The former case (vanishing outer loops) contributes to a constant flow stress increase, whereas the latter case (loop pile-up) contributes to work hardening. Both cases are quantified by discrete dislocation dynamics simulations using several particle distributions and grain sizes.

The indentation size effect and the arrangement of geometrically necessary dislocations

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Size effects in plasticity are well known since several decades (e.g. the Hall-Petch effect) and have gained more attraction in the last years due to micro-sample testing. The general process to realize plastic deformation in metals is the movement of dislocations. In order to accommodate plastic strain gradients, as are present beneath indents, dislocations of appropriate sign and character have to be stored in the crystal - they are so-called geometrically necessary dislocations. Usually, kinds of Nix-Gao models are used to describe the increasing hardness with decreasing indentation depth, which assume a self similar arrangement of geometrically necessary dislocations in the plastic zone. In order to prove this assumption and for a better understanding of phenomena involved in nanoindentation, detailed experimental analyses and discrete dislocation simulations of the size dependent evolution of the microstructure beneath indents have been performed.

The experimental studies are focused on the changes in crystal orientation caused by the indentation process, which can visualise the distribution of geometrically necessary dislocations. Cross-sections through the imprints and samples for transmission electron microscopy are prepared using the focused ion beam technique. Local crystal orientation changes determined by electron backscattering diffraction and direct observation of the dislocation structure beneath the imprints are used to get a closer insight into plastic processes during indentation. Additionally, discrete dislocation dynamics simulations are performed to get a feeling about the effect of dislocation source density, dislocation nucleation stress, lattice friction stress and the orientation of slip planes.

The experiments indicate pronounced differences in the developed orientation distribution for imprints smaller and larger than about 1 μm . This conflicts with the idea of a self-similar deformation behaviour in nanoindentation. The difference in the dislocation arrangement is reflected in the dependence of the hardness versus indentation depth dependence, too. Deformation mechanisms causing the observed changes in crystal orientation and their effect on the size dependence of hardness will be discussed.

Preference: Oral presentation

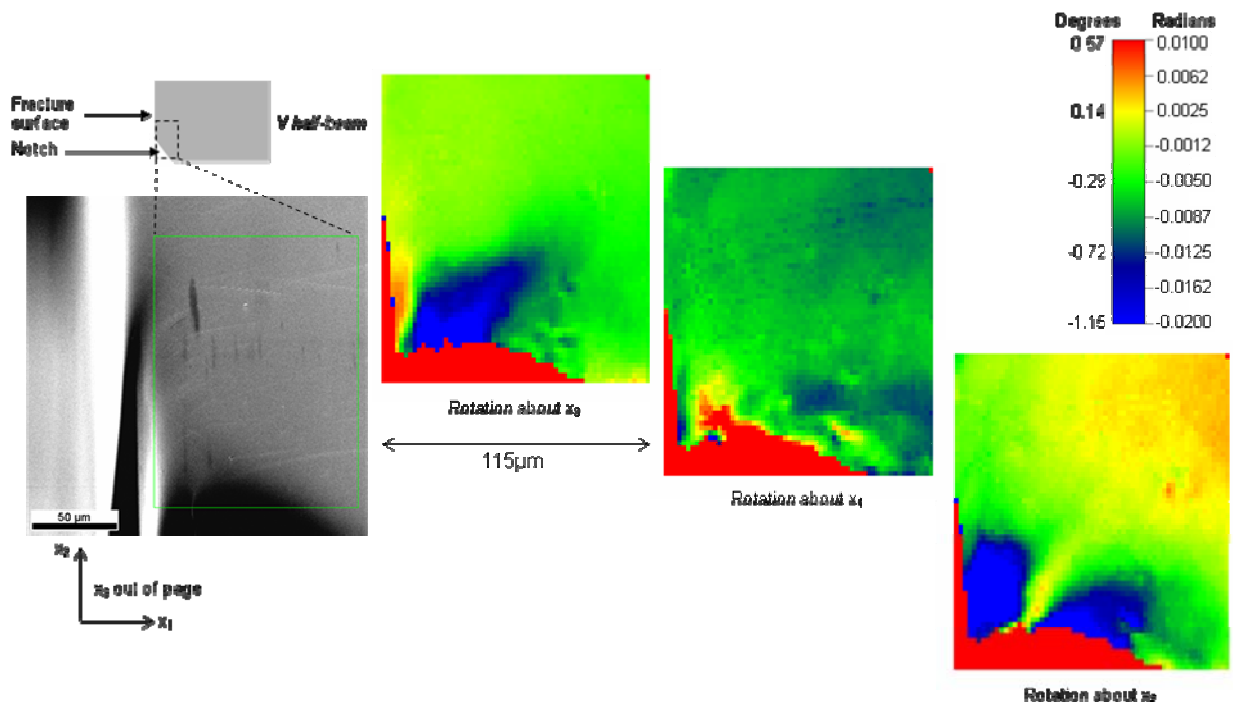
Presenter: Christian Motz

Characterisation of plastic zones around crack-tips in BCC metals using electron backscattered diffraction

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Interest in dislocation behaviour in BCC metals has recently increased, as many such metals are candidate materials for components in nuclear fusion reactors. Dislocation behaviour in BCC metals is relatively poorly understood compared to dislocation behaviour in FCC materials and conventional approaches to study dislocation behaviour in BCC materials have proved difficult. In this work, electron backscattered diffraction (EBSD) is used to map the deformation around intentionally-introduced cracks in various BCC metal single-crystals (tungsten, vanadium and iron). By analysing an array of several tens of thousands of Kikuchi patterns, very small rotations (<0.1 degrees) of the crystal lattice can be detected, as shown below for dislocations around a crack-tip in vanadium. The method allows the size and shape of the plastic zones to be deduced and consequently may allow an estimation of the mobility of dislocations in these metals. The experimental results obtained will be related to the latest findings of a modelling study of brittle-ductile transitions in these metals, also performed in Oxford.



Structure and behavior of basal dislocations in sapphire

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Sapphire represents a single crystal of alumina (α -Al₂O₃), which is one of the most widely used ceramics in industry due to the superior properties as a structural material, an insulator and so on. Accordingly, dislocations in sapphire have been intensely studied for past several decades. Basal dislocations play an important role in the high temperature deformation of sapphire since basal slip is easy slip system at elevated temperatures. It is known that a basal dislocation of $\mathbf{b}=1/3[11\bar{2}0]$ dissociates into two partials of $\mathbf{b}=1/3[10\bar{1}0]$ and $\mathbf{b}=1/3[10\bar{1}0]$. However, there were a lot of unclear points concerning the core structure of basal dislocations because of the lack of atomic scale analyses. In this presentation, we show the influence of the core structure of a basal dislocation on plasticity, diffusion and functional properties of sapphire, based on the observations by recent electron microscopy and high temperature deformation tests.

Studies of Plastic Deformation using Phenomenological Mesoscale Field Dislocation Mechanics

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Phenomenological Mesoscale Field Dislocation Mechanics is a continuum framework for the modeling of dislocation mediated plasticity. The approach results from averaging [1] a Field theory of Dislocation Mechanics [2] that adapts and generalizes formal elements of the theory of continuously distributed dislocations to develop a well-set, 3-d, PDE theory of coupled dislocation transport and internal stress. The averaging of this nonlinear system introduces new terms that can be physically interpreted and require closure; such closure is naturally provided by well-tested models of rate-dependent (polycrystal) plasticity, thus forging a rigorous link between the classical theory of dislocations and the theory of plasticity. The direct treatment of the transport of polar dislocation density combined with such closure presents a setting rather similar to the Large Eddy Simulation (LES) procedures for the Navier-Stokes equations – a resemblance that extends to the rich dynamical features of non-linear transport phenomena. The development of internal stress and propagation of plastic fronts follow naturally, without any local constitutive construction, by virtue of the internal stress and transport associated with the polar density. Large-scale applications are addressed through an implementation that brings together appropriate numerical algorithms, parallel coding strategies, and rigorous verification. To date, studies have been conducted on the creep of ice single crystals [3], propagation of Lüder's fronts [4], suppression of the yield point upon reversal of loading [5], and the Portevin-LeChatelier effect in single crystals. This present effort will review these applications. Subsequent attention will be turned to the size effect associated with the source generation of mobile dislocation density. Size effect will be demonstrated through both gradients inherent in the problem specification (torsion) and arrangement of dislocation sources.

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Dislocation transport in crystal plasticity

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Transport is a convective process by which certain species, or variations in certain quantities, propagate in a medium. It is pervasive in many branches of physics. For example, transport serves as a cornerstone in the theory of fluid dynamics. Crystal plasticity is due to motion of the linear lattice defects known as dislocations through the lattice. When dislocations are envisioned through their areal densities, their motion can be cast into the transport of these densities [1]. The resulting equation has been known for half a century, mostly as a curiosity, and it is only recently that it has been effectively used for dislocation dynamics predictions [2]. Known as the transport equation for dislocation densities, it has not received experimental validation yet, although several observations [3] could perhaps have been used in that aim.

Intermittency of plastic activity has been known for an even longer period of time [4]. However, until recently, the prevailing interpretation has been that, in average, over sufficiently large space and time scales, fluctuations in plastic activity statistically offset to a net smooth, homogeneous and stochastic overall response. It is only when statistical analyzes of these fluctuations became available, in particular from the determination of velocity fields in *Cu* single crystals oriented for multiple slip in tension [5], and when power-law distributions were repeatedly observed that it was realized that the dynamic nature of intermittency could be that of a critical scale-free phenomenon with long-distance spatial correlations.

In this presentation, it is our objective to evidence dislocation transport from observations of *Cu* single crystals at the adequate scale of observation, *i.e.* in the $\mu m - mm$ scale, to show its intimate connections with the intermittency of plasticity, and to substantiate these notions by giving an interpretation within the framework of a field dislocations mechanics theory [2]. It is shown that this theory, which combines dislocation transport and long-range internal stress field development, allows accounting for the heterogeneity and intermittency of plasticity, as well as for the observed spatio-temporal correlations.

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Preference: Oral presentation

Presenter: C. Fressengeas or A.J. Beaudoin

**The Orowan mechanism and its composition with forest hardening in ferrite:
a DD simulation study**

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A three-dimensional Dislocation Dynamics (DD) simulation is used to study the strengthening associates to the incoherent carbides included in the ferrite phase of Reactor Pressure Vessel (RPV) steel. Precipitation-induced strengthening is first investigated with a random distribution of spherical carbides alike the microstructures observed in RPV steel. In this case, strengthening can be predicted with simple relations accounting for the carbides distribution properties and the accumulation of Orowan loops. In a second step, a large density of dislocations (10^{14} m^{-2}) is incorporated in the reference volume. Latent hardening and tensile tests modeling are then proceed to investigate the non-trivial problem of precipitates and forest hardening composition. Demonstration is made that a quadratic mixture law can successfully reproduce the flow stress amplitudes we obtain in the DD calculations.

Deformation luminescence of X-irradiated KCl:Eu²⁺ by bending test

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It is well known that luminescence occurs during plastic deformation of X-irradiated alkali halide crystals. The luminescence is caused by dislocation motion. The luminescence gives us information about dislocation motion during deformation of a crystal. We carried out bending test of X-irradiated KCl single crystals doped with europium. The europium is known as a fluorescent material and is expected to cause strong luminescence. It allows us to observe light emission pattern from the sample by using a CCD camera.

Samples were cleaved out of an ingot of KCl crystal grown by Bridgman method. The size of samples was 1x2x12mm³. The samples were annealed at 1033K for six hours followed by slow cooling to room temperature. Samples were held at 623K for 30 minutes and then were quenched to disperse europium into the sample. They were exposed to X-ray before bending test.

Luminescence happens in the vicinity of the point where a central wedge touches the surface of a specimen and in that of the opposite side in the beginning of deformation. Several luminescence lines run along slip bands toward neutral axis from the surface. Then many luminescence lines intersect each other. Flash sometimes occurs both in the tension area and in the compression one. As deformation proceeds the luminescence lines are confused and right triangle-like luminescence pattern appears on both sides of the touch point of the wedge in the compression area as well as in the tension one. Strong flash takes place in the triangle-like area just before fracture and there then occurs fracture.

Interaction between dislocation and divalent impurities in KBr single crystals

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Japan.

Divalent impurity in alkali halide crystal turns into I-V dipole, combining with positive vacancy. The I-V dipole has tetragonal stress field in the crystal. It is known that the tetragonal stress field interacts screw dislocation and makes the crystal hard. It is reported that we can obtain the interaction profile between dislocation and weak obstacle by measuring the strain rate sensitivity under superimposition of oscillatory stress during plastic deformation. Stress decrement due to oscillation and stress change due to strain rate cycling have been measured during plastic deformation of KBr single crystals doped with Mg^{2+} , Ca^{2+} , Sr^{2+} or Ba^{2+} . The relation between the strain rate sensitivity (SRS) of flow stress and stress decrement has a stair-like shape and is divided into three regions. The first region is a plateau at the small stress decrement, followed by gradually decreasing region (second) and subsequent plateau region (third). The stress decrement (τ) at the first bending point between the first and second regions is considered to be the effective stress due to impurity. The difference (λ) between SRS in the first and second plateau regions is also considered to be a part of SRS due to impurity. τ and λ were measured in the temperature range from 77K to room temperature. τ increases with decreasing temperature for every kind of KBr and the temperature that τ becomes 0 increases with increasing ionic radius of the divalent ion. The relation between τ and activation volume obtained from the λ reveals the interaction between dislocation and impurity. The Barnett relation is assumed to be applicable to the case of KBr crystals doped with divalent impurity. Then, the interaction energies between dislocation and Mg^{2+} , Ca^{2+} , Sr^{2+} and Ba^{2+} were determined to be 0.36, 0.23, 0.30 and 0.58eV in KBr, respectively.

Optical properties of dislocations in wurtzite ZnO single-crystals

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Wurtzite ZnO bulk single-crystals were compressively deformed at elevated temperatures 923 - 1123 K to introduce a number of fresh dislocations with the Burgers vector of $a/3\langle 11\bar{2}0 \rangle$. ZnO, including a high density (more than 10^9 cm^{-2}) of dislocations, showed photoluminescence (PL) light emission lines with photon energies of 3.100 eV and 3.345 eV, as well as their LO-phonon replicas, at a temperature of 11 K, and the intensities increased with increasing dislocation density. The higher the light intensity was, the lower the deformation temperature was. These results and the optical data obtained by temperature-dependent PL and excitation-power dependent PL suggest that point defect complexes involving dislocations gave rise to these emission lines.

Solid Solution Hardening in faced centred binary alloys

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We report our atomistic study on the solid solution hardening SSH in faced centred binary alloys, exemplified by 2 alloy models, i.e. Ni(Al) and Al(Mg) prototypical of large and small size misfits, respectively. We demonstrate that both types of dislocation, edge and screw experience similar pinning strength mainly due to the short range interaction between the in-plane solutes and the dislocation partial cores. We computed the pinning strength for different obstacles, i.e. either single isolated impurities at different position around the glide plane or solute dimer with different orientation and position. The pinning strength of an obstacle is shown to be of the order or less than $0.05\mu b^2$ and varies strongly with the obstacle position and the dimer bound direction. The interaction can be either repulsive or attractive depending on the position inside or outside the stacking fault. The predictions of the different analytical models for SSH are compared to our atomistic simulations.

Anomalous mobility of dislocation kink solitons in disordered solid solutions

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Dislocation kink solitons in disordered solid solutions provide an example of quasiparticles showing anomalous kinetics—i.e., the nonlinear dependence of the displacement x on the time t , $x \sim t^\delta$. To describe the dynamic phase transition from the ordinary linear to anomalous regime, the dynamics of a quasiparticle in an energy landscape that performs a correlated random walk on the energy scale was theoretically studied. The phase diagram was characterized by the calculated temperature dependence of the threshold driving force F_{th} below which the average velocity of quasiparticles vanishes. The exponent δ of the kinetic equation for the anomalous phase, $x \sim t^\delta$, was determined by simple statistical arguments using the concepts of the “optimal fluctuation method.” The dependence of the threshold driving force F_{th} on the concentration of solute atoms and statistical properties of a random energy landscape relevant to disordered solid solutions was calculated. The correlations between steps of the random potential were shown to modify the concentration dependence of F_{th} , thereby providing a qualitative explanation of experimental data on the dislocation pinning in solid solutions.

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Ab-initio Calculations of Screw Dislocations in Tungsten and Tungsten-Re Alloys

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Tungsten is the metal with the highest melting point and is, therefore, a promising material for a wide range of technological applications where components are facing high temperatures. A major drawback in this connection is, however, the ductile to brittle transition which for tungsten occurs above room temperature. Alloying with rhenium is known to improve the ductility of the crystal, where the reasons for this have, however, not yet been clarified. While many effects could be important in this connection, a prominent role is associated to the fundamental properties of screw dislocations.

In this contribution we present density functional theory calculations of $\frac{1}{2} \langle 111 \rangle$ screw dislocation dipoles. Special attention is given to the core structure, the core energy, and to the Peierls stress. The influences which occur upon alloying are investigated by means of the virtual crystal approximation.

Dynamic Dislocation-Defect Analysis: Forest Dislocations, Solutes, Clusters and Transition Phases

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Thermally activated plastic flow of crystalline solids has had a long history since the discovery of the Cottrell-Stokes relation. The theoretical analyses have been well documented and recent reviews have affirmed the earlier interpretation of the data. The problem has been the precision of the measurement of the activation volumes and how to not only account for crystalline defects such as forest dislocations and deformation debris but also obstacles intrinsic in the lattice. Moreover the activation volume is comprised of two independent parameters which are the inter-obstacle spacing and the activation distance. Over the last two decades our development of precision strain rate sensitivity has enabled the precise determination of the activation volume. Furthermore it was shown that the up-strain-rate change measures the dislocation-forest intersection whereas the down-rate change, that of the forest plus that of debris for pure metal systems. The recent dynamic dislocation-defect analysis permits a re-examination of the stress-strain relation together with the activation volume and the mean slip distance. This analyses results in an activation-distance prediction diagram which can determine this parameter without invoking the flow stress to assess the inter-obstacle length. Thus this analysis permits the characterization of the thermodynamic controlling mechanism for any given microstructural state, whether they are supersaturated solid solutions or their decomposed state. This study shows that although the activation distance, measured in fractions of Burgers vectors dependent on the temperature, may remain constant, the strain rate sensitivity can vary greatly with strain. This effect has been shown to depend on the degree of dynamic point-defect supersaturation due to its generation and annihilation at available sinks. The understanding of this phenomenon is important in fabricating products from alloy sheets.

Discrete transformation-dislocation model

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A discrete model for analyzing the interaction between plastic flow and martensitic phase transformations is developed. The model is intended for simulating the microstructure evolution in a single crystal of austenite that transforms non-homogeneously into martensite. The plastic flow in the untransformed austenite is simulated using a plane-strain discrete dislocation model. The phase transformation is modeled via the nucleation and growth of discrete martensitic regions embedded in the austenitic single crystal. At each instant during loading, the coupled elasto-plasto-transformation problem is solved using the superposition of analytical solutions for the discrete dislocations and discrete transformation regions embedded in an infinite homogeneous medium and the numerical solution of a complementary problem used to enforce the actual boundary conditions and the heterogeneities in the medium. In order to describe the nucleation and growth of martensitic regions, a nucleation criterion and a kinetic law suitable for discrete regions are specified. The constitutive rules used in discrete dislocation simulations are supplemented with additional evolution rules to account for the phase transformation. To illustrate the basic features of the model, simulations of specimens under plane strain uniaxial extension and contraction are analyzed. The simulations indicate that plastic flow reduces the average stress at which transformation begins, but it also reduces the transformation rate when compared to benchmark simulations without plasticity. Furthermore, due to local stress fluctuations caused by dislocations, martensitic systems can be activated even though transformation would not appear to be favorable based on the average stress. Conversely, the simulations indicate that the plastic hardening behavior is influenced by the reduction of the effective austenitic grain size due to the evolution of transformation. During cyclic simulations, the coupled plasticity-transformation model predicts plastic deformations during unloading, with a significant increase in dislocation density. This information is relevant for the development of meso- and macroscopic elasto-plasto-transformation models.

Preference: Poster presentation

Presenter: Jingyi Shi

HRTEM observation of displacement fields around dislocations in quasicrystals

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Originating in the quasiperiodic translational order, quasicrystals have a special type of elastic degrees of freedom, termed as phason degrees of freedom. Dislocations in quasicrystals are generally accompanied by the phason displacement fields in addition to the conventional displacement fields[1]. According to a generalized elastic theory of quasicrystals, several groups have attempted to deduce analytical expressions of displacement fields around various types of dislocations in quasicrystals. In contrast, there have been no experimental studies of displacement fields around the quasicrystalline dislocations. In this study, we have observed the displacement fields by high-resolution transmission microscopy (HRTEM) and compared them with the theoretical displacement fields to examine the validity of the generalized elastic theory of quasicrystals. The effects of phason elastic constants on the displacement fields have been discussed and evaluation of their values has been attempted.

[1] For a review, see K. Edagawa and S. Takeuchi, '*Dislocation in Solids*' ed.By F. R. N. Nabarro and J. P. Hirth (Elsevier B. V. 2007), Chap.76, pp367

Preference: Poster presentation

Presenter: Yeong-Gi So

Dislocation Core Interaction in Low-angle Grain Boundaries of Alumina

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In this study, we systematically fabricated alumina (α -Al₂O₃) bicrystals with $\{11\bar{2}0\}/\langle 1\bar{1}00 \rangle$ low-angle grain boundaries. The grain boundary structures were mainly observed by high-resolution transmission electron microscopy (HRTEM). It was found that the grain boundaries consisted of the array of discrete dislocations. They were not the perfect dislocations with $\mathbf{b} = 1/3\langle 11\bar{2}0 \rangle$ perfect, but the partial dislocations with $\mathbf{b} = 1/3\langle 10\bar{1}0 \rangle$ and $\mathbf{b} = 1/3\langle 01\bar{1}0 \rangle$. The periodicity of the two pair partials can be explained by Frank's simple geometric model, but the separation distance between the two partials should be estimated by considering mutual interaction between the partial cores. In general, strain and stacking-fault energies can be considered to calculate the dissociation distance between the partials. However, our systematic study suggests that Coulomb interaction should be considered between the two partials. By precisely changing the misorientation and thus changing the dislocation distances with atomic-scale precision, the extra charge of the dislocation cores was estimated by the slight deviation in partial separation distances. The present findings are consistent with the recent report showing that the partial cores of alumina are locally nonstoichiometric [N. Shibata et al. Science **316** (2007)]. We will discuss the Coulomb interaction and the charging state of the dislocation cores in detail.

Preference: Poster presentation

Presenter: E. Tochigi

Dislocation based modeling of plasticity in superalloy single crystals: hybrid DD – FE simulations

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At high temperatures, single crystals of nickel-base γ/γ' superalloys exhibit excellent mechanical properties. The microstructure of these superalloys with high γ' phase volume fraction consists of regular cuboidal precipitates separated by narrow channels of the γ phase. In this microstructure, dislocation motions and reactions become complex processes and induce a specific orientation dependence of the critical resolved shear stress.

Simulations of Dislocation Dynamics (DD) in representative volume elements have the potential for correlating microstructural properties with the mechanical behavior of a large sample. For this reason, 3D simulations have been developed in which the boundary value problem is rigorously resolved through a coupled approach, involving a Finite Element code and a DD code: the Discrete–Continuous Model (DCM). This model takes into account: – the anti-phase boundary energy and the formation of superdislocations in γ' precipitates, – the anomalous temperature dependence of the mobility of superdislocations in the γ' phase and – the presence of misfit stresses at the γ/γ' interphases.

Different loading conditions are tested in order to investigate collective phenomena and microstructural mechanisms at the origin of the strain localization in coarse slip bands. In particular, analyses of both formation and evolution of the dislocation microstructures in oriented specimens near $\langle 111 \rangle$ -oriented specimens can explain the deformation which is experimentally observed along the cube planes. The DCM results are finally compared with the predictions of a continuum model based on dislocation densities. Special attention is paid to the process of storage of geometrically necessary dislocations at the γ/γ' interphases.

Preference: Oral presentation

Presenter: Aurélien Vattré

Core Structure, Peierls Potential and Kinks of Screw Dislocations in α -Fe from First Principles

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A quantitative description of straight and kinked $\langle 111 \rangle$ screw dislocations in iron from first principles is presented. The calculations are carried out within the density functional theory (DFT) framework using the SIESTA code and simulation cells containing up to 800 atoms. The construction of simulation cells appropriate for such extended defects has been optimized for cell sizes accessible to DFT calculations. We have rationalized the cell-size dependences of the energetics evidenced both in the cluster approach and in the dipole approach for various cell and dipole vectors; they are due respectively to surface-dislocation and core-core interactions. It is concluded that a quadrupolar arrangement of dislocation dipoles is best suited for such calculations.

In agreement with previous DFT calculations in body centered cubic metals, a non-degenerate structure is found for the core. From a detailed comparison with anisotropic elasticity a significant dilation effect has been evidenced in addition to the Volterra field. Two high symmetry directions of the Peierls potential have been sampled: the line joining two easy-core positions – which gives the Peierls barrier – and that from an easy to a hard-core position. The behavior of the Ackland-Mendelev potential for iron, which gives the correct non-degenerate core structure unlike most other potentials, has been tested against the present results. It compares well with the DFT results for the γ -surfaces but discrepancies appear on the deviation from anisotropic elasticity of the edge component and on the Peierls potential: it underestimates the Peierls energy by a factor of three and overestimates the energy difference between easy and hard cores by a factor of five, and it yields a double-hump Peierls barrier instead of a single hump one within DFT. Attempts to improve this potential will be presented.

Finally, the structure and the formation and migration energies of single kinks have been investigated. The methodology for constructing triperiodic cells with a single kink on each dislocation line has been developed. Results obtained with empirical potentials as well as preliminary DFT calculations are presented. The two types of kinks – left and right – are found to have significantly different formation energies.

Formation of point defect by dislocation reaction in some metals and intermetallic compounds

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Point defects in metals and intermetallic compounds may have important effects on their properties, such as strength, ductility, fatigue and high temperature creep, due to their movement and interactions with dislocations and other defects during deformation. Molecular dynamics simulation were carried out to elucidate the formation mechanism of various kind of defects in metals, including Ti, Al, Cu and some intermetallic compounds, such as TiAl. It was found that different defects, such as vacancy, self interstitial atoms can be formed by dislocation reaction of different configuration during plastic deformation. The point defects can further rearrange themselves and form defect clusters in different form such as dislocation loops of interstitial or vacancy type. The formation process and atomic structures of each kind of defects were characterized. The influence of these point defects to the dislocation movement and deformation behavior was studied. It was shown that the defects can react with dislocation and strongly influence its motion when they exist on the same slip plane, and will slow down or pin down the moving dislocation when they are on nearby slip plane, depending on the nature of defects and the distance between the slip planes.

Deformation Defects: from Dislocations to Plasticity Localization Waves

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Conventional dislocation approaches used by addressing plastic flow are re-considered in the light of a new wave concept of deformation macro-localization. Holographic investigations were performed for single- and polycrystalline fcc, bcc and hcp metals and alloys. Plastic flow regularities are found to occur from yield limit to failure as macro-localization patterns. Experimental evidence indicates that dislocation shears are activated successively to give 5...10 mobile or stationary spatially correlated domains; these have non-uniform deformation field of their own and are regarded as specific macro-scale defects. A space-time localization pattern results from dislocation self-organization; this has wave features, i.e. length $5 < \lambda < 10\text{mm}$ and rate $10^{-5} < V < 10^{-4}\text{m/s}$. A two-component model of plastic flow self-organization is proposed, which is based on the interaction of the crystal's phonon and dislocation sub-systems. This reconciles commonly known dislocation mechanisms acting at the various deformation hardening stages in single crystals and accounts for the above regularities of wave generation. The basic assumptions of the model are as follows. Relaxation-type plasticity involves dislocation acts that generate acoustic emission pulses causing elastic energy re-distribution among the stress concentrators (dislocations). As a result, the stresses at the concentrators grow to initiate their relaxation by dislocation shears. The sequence of events is repeated. For relaxation events to be activated, stress concentrators of the same type and size must be initiated, which is provided by acoustic pulses of strictly specified shape and spectrum, their amplitude being less significant. Thus, the concepts of defect self-organization and of energy re-distribution among stress concentrators involved successively in relaxation acts, might help account for the low values of localization wave rate and for the large-scale correlations of localization domains occurring in a deforming system that only contains micro-scale defects (dislocations).

Plastic deformation of silicon wafer to shaped-crystal

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In semiconductor industries dislocations and plastic deformation are recognized to be unlike not only for slip and warpage of wafers during device processing but also for causing inhomogeneities/degradation of optical and electronic functionalities. Therefore, for nearly forty years extensive researches have addressed fundamental knowledge on the dislocation motion and plastic deformation of semiconductor materials in order to eliminate, suppress and control of dislocation motion and plastic deformation. However, in a viewpoint of materials processing plastic deformation to an arbitrary shape beyond two dimension products is important for wide applications even of semiconductor materials. Indeed, successful production of Si optical lenses has been reported recently [K. Nakajima et al., *Nature Materials* **4** (2005) 47]. We herein report on dislocation characters in Si wafer bended at elevated temperatures for understanding dislocation dynamics during such wafer deformation process.

Si wafers can be deformed to a concave/convex shape by bending with hemisphere dies at temperatures higher than 1100°C. Etch pits of dislocations induced by the bending distribute inhomogeneously, showing four-fold and six-fold patterns with high etch pit density wings along the $\langle 1\bar{1}0 \rangle$ directions in (100) and (111) wafers, respectively. Also, etch pit density is 10^8 cm^{-2} in the wafer central region and 10^4 cm^{-2} in the wafer periphery, showing expansion of the plastically deformed region from the central region during the wafer bending process. Wafer bending process should be discussed in terms of motion and mutual interaction of dislocations in multiple-activated slip systems under spatial stress variations.

Resolving the geometrically necessary dislocation content in zircon by conventional EBSD

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The deformation-related microstructure of an Indian Ocean zircon (hosted in a gabbro deformed at amphibolite-grade) has been quantified by conventional electron backscatter diffraction. Orientation mapping reveals progressive variations in intragrain crystallographic orientations that accommodate orientation differences up to 20° within the zircon crystal. These variations are manifest by discrete low angle boundaries that separate domains recording no resolvable orientation variation.

From the orientation data gathered on a regular grid on the surface of the specimen, the local lattice curvatures are determined and six components of the curvature tensor are resolved. Neglecting any possible elastic strain gradients, five components of the local dislocation density tensor and one independent difference between two other components are determined and, hence, substantially more information extracted, than the hitherto reported three components. For a decomposition of Nye's dislocation density tensor into individual dislocation types, edge and screw dislocations with Burgers $[100]a$, $[010]a$ or $[001]c$ and line vectors along the coordinate axes are considered, because of the tetragonal symmetry of zircon. Taking into account the anisotropic elastic constants, the most favourable dislocation configuration is found by minimizing the total dislocation line energy.

The resolved geometrically necessary dislocation content is sufficiently high to have a marked effect on the geochemical behaviour of zircon, via enhanced bulk diffusion and increased dissolution rates. Therefore, crystal plasticity in natural zircon may have significant implications for using zircon for interpretation of radiometric ages.

Oral presentation preferred

Dislocation activity within nanocrystalline metals: a molecular dynamics study

C. Brandl, E. Bitzek, P. M. Derlet, H. Van Swygenhoven

The use of large scale molecular dynamics to study the mechanical properties of FCC nanocrystalline (nc) metals provides a detailed picture of the atomic-scale processes during plastic deformation at room temperature. Simulations have revealed interface dominated processes such as grain boundary sliding and migration, and intragranular deformation processes involving dislocation activity. In particular grain boundaries can act as both sources and sinks for partial or full dislocations and that the surrounding grain boundary environment can significantly affect the motion of a dislocation as it propagates through the grain (Acta Mater. 54, 1975 (2006)). Simulations have now revealed that cross-slip via the Fleischer mechanism also occurs in nc-Al simulations, and that the grain boundary structure is found to strongly influence when and where cross-slip occurs, allowing the dislocation to avoid local stress concentrations that otherwise can act as strong pinning sites for dislocation propagation. More generally, a statistical analysis of dislocation activity as a function of strain up to 9% total strain has been performed. From such an analysis it emerges that (1) measurable slip is only observed beyond the maximum flow stress whereas dislocation nucleation occurs at lower stresses indicating that propagation is the rate limiting process in simulation, (2) the resolved stress at which a slip event can be correlated with the underlying dislocation process and (3) there is a distribution of critical resolved shear stresses needed to describe slip. These results are discussed in the framework of realistic micromechanic models for nanocrystal plasticity.

Phase Field Modelling of Stacking Fault Shear in Nickel Base Superalloys

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Results obtained using a Phase Field Model (PFM) describing dislocation propagation in a simulated nickel base superalloy will be presented. The model is used to examine the movement of dislocations through the $L1_2$ ordered superalloy. In particular, the cutting of γ' precipitates by γ matrix dislocations has been studied with the aim of verifying the governing mechanisms of primary creep. Formation of nodes and networks has also been examined. The model demonstrates various dislocation reactions, such as recombination, reordering and annihilation. The formation and evolution of superlattice and complex stacking faults and anti-phase boundaries is achieved by incorporating fault energy data (gamma surfaces) obtained from Molecular Dynamics (MD) simulations. The observed likelihood of stacking fault formation is found to exhibit a strong stress dependence. The simulated stacking faults form less readily as the applied stress approaches the superalloy's theoretical yield. This may help demonstrate why stacking faults are observed in specimens that have undergone creep and not in those subjected to a simple tensile test.

Interaction of an edge dislocation with $\frac{1}{2}\langle 111 \rangle$ and $\langle 100 \rangle$ dislocation loops in α -Fe : an atomistic study

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Abstract

Microstructure of irradiated Fe and ferritic Fe-based alloys typically consists of dislocation loops, small clusters of vacancies and, in some cases, second phase particles. Dislocation loops visible in a TEM are mostly interstitial-type loops with Burgers vector \mathbf{b} equal to either $\frac{1}{2}\langle 111 \rangle$ or $\langle 100 \rangle$. The presence of these loops in the matrix obstructs motion of dislocations, leading to an increase in the yield stress and reduction in ductility. Furthermore, experimental observations suggest that the ability of dislocations to absorb these loops assists in the formation of defect-free channels, which may cause plastic instability and loss of work hardening. It is therefore important to understand mechanisms of interaction between the loops and dislocations.

Molecular dynamics simulations were used to investigate reactions between an edge dislocation with $\mathbf{b} = \frac{1}{2}\langle 111 \rangle$ and interstitial dislocation loops with \mathbf{b} equal to either $\frac{1}{2}\langle 111 \rangle$ or $\langle 100 \rangle$ at different locations with respect to the slip plane. The loop size was varied from 0.5 nm up to 10 nm, and simulations of both static ($T = 0\text{K}$) and dynamic ($T > 0\text{K}$) conditions were performed. The results show that small loops (with size up to 1nm) are absorbed on the dislocation, independently of their \mathbf{b} . Large loops are strong obstacles and, depending on the mutual orientation of the dislocation and loop Burgers vectors, are either completely or partially absorbed. The obstacle strength and reaction product depend on T and are controlled by the mobility of either the dislocation segment formed in a favourable loop-dislocation reaction or screw segments in a dipole drawn out on the pinned dislocation.

Strengthening due to Cr precipitates in Fe-Cr alloys : theory vs. atomistic simulations

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Abstract

FeCr alloys are the base matrix of high-Cr ferritic/martensitic (FM) steels for industrial applications. FeCr binary alloys as well as FM steels exhibit α - α' phase separation, if Cr content exceeds 10%at., resulting in the formation of fine-dispersed nano-meter size precipitates, in the range of temperatures relevant for technological applications (500-900K). This precipitates obstruct motion of dislocations leading to additional hardening and risk of embrittlement. In order to develop predictive models of hardening and embrittlement of aged steels it is important to quantify precipitate-dislocation interaction in terms of critical stress and its temperature dependence.

In the present work, we apply molecular dynamics (MD) techniques to study the interaction of dislocations with Cr precipitates of different sizes at different temperatures in Fe-10Cr matrix (typical content of Cr in FM steels). The corresponding stress-strain curves are thereby obtained and the mechanisms of reactions are investigated. Theoretical models based on elasticity theory, which account for different strengthening mechanisms (size-misfit, modulus misfit and chemical strengthening) are applied, being parameterized using the interatomic potentials. The ultimate goal of the work is to confront the data obtained using both theoretical and simulation methods and thus to reveal prevailing mechanism of precipitate strengthening in Fe-Cr alloys. Another aspect is the thermal activation parameters, which can be also extracted from MD simulations, and can be compared with phenomenological models based on experimental results (meaning p and q) .

ECCI Observation of Dislocation Structures around Fatigue Cracks in Ferritic Stainless Steel Single Crystals

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Dislocation structures around crack tips — which are difficult to be investigated by transmission electron microscopy — were observed with electron channelling contrast imaging (ECCI) method. The ECCI method enables us to observe dislocations lying near surface using a scanning electron microscope.

Compact tension specimens having $20 \times 20 \times 2 \text{ mm}^3$ shape were cut from an Fe-30%Cr alloy single crystal which was grown by Bridgman method. Loading axes of the specimens were $\langle 112 \rangle$, $\langle 111 \rangle$, $\langle 221 \rangle$ and $\langle 110 \rangle$. Fatigue crack growth tests were carried out in air at room temperature. For the ECCI observation, the surfaces of the cracked specimens were polished to obtained smooth surface. The ECCI observation was conducted using JEOL JSM-6500F FE-SEM.

The propagating fatigue cracks were classified into two types from shape of crack surface: one had sinusoidal crack surface and the other had flat one. The fatigued specimens having the $\langle 112 \rangle$, $\langle 111 \rangle$ and $\langle 221 \rangle$ loading axes usually exhibited the propagations of the sinusoidal cracks. On the other hand, the flat cracks were seen in the specimen with the $\langle 110 \rangle$ loading axis.

In the vicinity of the sinusoidal cracks, cell structure was locally detected by the ECCI observation. On the outer side of the cell structure area, vein dislocation structure was developed. On the other hand, the ECCI observations of the flat cracks revealed that the cell structure was almost absent even near the crack surface. Hence, it is suggested that the shape of the crack surface was associated with the surrounding dislocation structure.

A Dislocation-Based Approach to Identify Fracture Process

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Microstructures near fracture surfaces of copper specimens tested under monotonic and fatigue deformation were investigated using electron channelling contrast imaging (ECCI) method and electron backscatter diffraction (EBSD) analysis. With the ECCI method using a scanning electron microscope, we can observe dislocation structures through a wide area. The purpose of the present study is to find new criteria for identification of fracture process instead of the conventional fractographic technique.

A monotonic tensile test and a fatigue test were carried out in strip specimens of polycrystalline copper. Stress amplitude of the fatigue test was 80MPa. The fatigued specimen was fractured at 1.1×10^6 cycles. After the specimens were fractured, the microstructures near fracture surface were observed by the ECCI method using JEOL JSM 6500F FE-SEM. Crystallographic orientations of the same areas were also analyzed by TSL OIMTM system.

Near the fracture surface of the specimen subjected to monotonic deformation, mottled patterns with sinusoidal edges were observed with the ECCI method. This pattern should be due to frequent change of crystallographic orientation. The frequent orientation change and high-density low angle boundaries were confirmed by the EBSD analysis. On the other hand, the ECCI observation revealed that cell structure was formed in the vicinity of the fracture surface of the fatigued specimen. At region distant from the fracture surface, “vein” and “ladder-like” dislocation structures, which are peculiar to fatigue deformation. In the EBSD analysis, grain distortion in the fatigued specimen was significantly small in comparison with the fracture under the monotonic deformation. Accordingly, it is suggested that the ECCI observation should be helpful in fracture analysis.

HARDNESS AND DEFORMATION MECHANISMS OF Ti_3SnC_2 STUDIED BY NANOINDENTATION AND AFM

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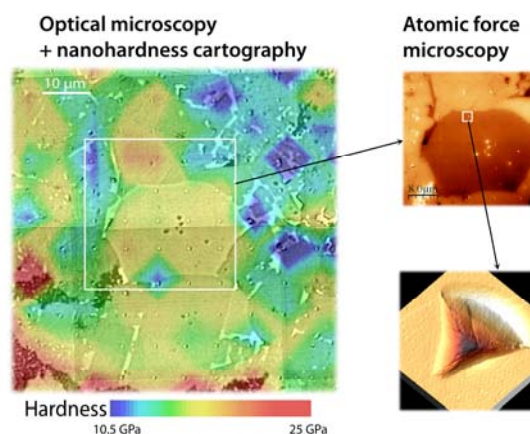
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The ternary $\text{M}_{n+1}\text{AX}_n$ carbides and nitrides compounds have recently aroused great interest due to their outstanding properties. In these compounds M denotes an early transition metal, A is an A-group element (from IIIA to VIA) and X is either C or N. The metallic nature of the bonding and the nano-layered nature of the structure give rise to a unique combination of metallic and ceramic properties. However, a rather low hardness value (2-5 GPa) is often reported for this material.

In this study, Hardness and Young's modulus of Ti_3SnC_2 , a recently synthesized MAX phase, has been determined by nanoindentation. The tested sample was composed of 80.5% of the MAX-phase Ti_3SnC_2 , 16.2% of TiC, 0.3% of FeSn, 0.8% of FeSn_2 and 2.2% of Sn. Due to the complex nature of the sample, a statistic analysis has been performed over 400 indents, organised in a regular square shaped array, with a step size of $7\mu\text{m}$. In particular, a hardness cartography has been established and superimposed to an optical microscopy image of the sample. In this way, the different hardness values have been related to the different phases but also to the different Ti_3SnC_2 grains. The grain orientations have then been determined by electron back scattering diffraction (EBSD), and a strong correlation has been found between hardness and grain orientation in Ti_3SnC_2 .

The surface deformations generated around the indents have then been observed by atomic force microscopy (AFM). Delamination and slip lines have been observed. For some grain orientations, the deformation could be explained by dislocation glide in the basal plane and by kink bands formation. For some other orientations, evidences of dislocation glide out of the basal plane and cross slip are observed.



POP-IN PHENOMENON AND NUCLEATION OF DISLOCATIONS DURING NANOINDENTATION IN MgO

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The pop-in phenomenon is a discontinuity often observed on nanoindentation curves. It corresponds to an abrupt increase in penetration depth without increasing the load. This phenomenon is observed in many materials during loading and sometimes during unloading. Most of the time, the deformation before the apparition of the pop-in is entirely reversible. For this reason, the pop-in is commonly associated to the nucleation of the first dislocations in the tested material. This hypothesis is supported by the fact that the deformed volumes are so small that they can be considered as exempt of pre-existing dislocations. Furthermore, the stress induced by the indenter can reach values close to the theoretical strength of the material. But the mechanisms of dislocation nucleation are still misunderstood.

In this study, nanoindentations have been performed in magnesium oxide (MgO) single crystals with a spherical indenter (radius: 10 μm), and the dislocation structures around the indent have been revealed by AFM and by the nanoetching technique. It is shown that with a careful surface preparation, reversible deformation can be achieved for indentation load higher than 300 mN. However, for some of these reversible indentations, pile ups of few dislocations are observed in the indented area, even if no pop-in occurred during the indentation. These observations suggest that the reversible deformation before the pop-in may involve dislocations. This hypothesis is discussed and compared to the resolved shear stress generated by the indenter during loading and unloading.

To determine the homogeneous or heterogeneous nature of dislocation nucleation during nanoindentation in MgO, nanoindentations have been performed in helium implanted MgO single crystals. The influence of the vacancy concentration on the dislocations behavior (nucleation and propagation) is discussed.

DIRECT EVIDENCE FOR THE KEY ROLE OF DISLOCATION MECHANISMS IN WORK HARDENING OF SINGLE UP TO NANOSTRUCTURED CRYSTALS UNDER INTERNAL FRICTION, FATIGUE AND SHOCK LOADINGS

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This work is the first direct evidence for the universal key role of individual dislocation mechanisms in all types of crystals and at all stresses along the deformation curve from internal friction ($\varepsilon \sim 10^{-8}$) up to nanostructured and fractured crystals (NSC). The effect of interrupted quasi-static, impulse and shock compressive/extension stresses, τ ($\tau = 0.6\tau_0$ to $95\tau_0$, where τ_0 is the resolved shear stress) and stress rates (10 to 10^6 MPa/sec) on dislocation dynamics was investigated in pure NaCl and InSb single crystals (SC) in the temperature range $T = 0.004$ to $0.945 T_{\text{melt}}$, T_{melt} is the melting point. It is shown that the jumping and damping motion of dislocation groups and serrated macroflow are of the same origin, and they are determined by the correlated cross-slip, conservative motion of jogs-superkinks, climb of jogs (with lattice defects production) and the Orowan bowing of superkinks-segments between the pinning points (jogs-impurity precipitates, dislocations, etc.) under external stress. Having covered a certain ultimate mean path lengths of individual dislocations determined by the pinned jogs of cross-slips (due to crystal prehistory and test parameters), the dislocation groups exposed to successive acts of multiplication thus forming the slip lines, bands, low/high-angle/nanograin boundaries. The same mechanisms explain the double correlated relaxation peaks of internal friction (Niblett-Wilks – Bordoni, Hasiguti, Ke-Mash-Hall and NSC recrystallization), the macroscopic recrystallization in NSC. The scaling of the flow stresses for dislocation motion, multiplication and deformation at fixed strains in SC and NSC up to fracture and the same temperature dependences of activation energies and activation volumes [1] confirms the above conclusions.

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NEW EVIDENCES FOR THE DEFORMATION ORIGIN OF INSULATOR-METAL-SUPERCONDUCTOR, NORMAL-SUPERFLUID TRANSITIONS

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The works [1-4] directly evidence for the key role of deformation in phase transitions (PT) and electrons in dislocation double cross-slip (DDCS). These data mean that single electrons and Cooper's pairs make the additional DDCS at very low temperatures due to lattice strains around the charges (the so-called phonons) which determine electrical impedance. And it is the sharp changes in temperature, hydrostatic pressure, deformation, particle irradiation, etc, which induce higher stiffness of various materials (under cooling, irradiation, etc.) that is the cause of normal-to-superconducting (superfluid) transition due to the abrupt drop of matrix drag for the particles flow. This consideration allows one to treat the current-voltage plots as the stress-strain curves where the Hook's law before the plastic flow is identical to the Ohm's law for electric current, the influence of magnetic field on the plastic properties of solids and liquids (the so-called magnetoplastic effect) explains the effects of orientation of electromagnetic field, amplitude, frequency on normal and superconductivity (superfluidity), PT, etc. This is confirmed by the extradeep penetration of high velocity cast iron microparticles into steel target at 77K in comparison with room-temperature data [5] and deformation physical-chemical effects at PT.

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THE SAME KEY MECHANISMS OF SERRATED FLOW OF CRYSTALS ALONG THE DEFORMATION CURVES IN THE RANGE FROM $\varepsilon \sim 10^{-8}$ TO $\varepsilon \leq 10^3$

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At all types of successively applied compressive and compressive-tensile stresses $\tau \sim (0.5-6.3)\tau_0$, τ_0 is the resolved shear stress, with various stress rates $d\tau/dt \sim 10^{-3}$ to 10^7 MPa/s (internal friction loadings with $f=100$ kHz are included) the dislocation motion and multiplication in pure and impure alkali-halides and semiconductors are defined by various contribution of a conservative and nonconservative motion of jogs, formed at dislocation double cross-slips, Orowan bowing of dislocation segments-superkinks between jogs and impurity microprecipitates and climb of dislocations in the temperature range $T = 4 \cdot 10^{-3}$ to $0.6 T_{\text{melt}}$, T_{melt} is the melting point. It is well known that the deformation of crystals usually gives rise to a much smaller number of intrinsic interstitials than vacancies provides direct evidence for the conservative motion of the preferentially interstitial jogs along the screw dislocations to the different obstacles [1]. This fact well explains the lower temperature relaxation peak (TRP) due to dominant conservative and higher TRP due to dominant non-conservative motion of jogs-superkinks, the double low-temperature (Niblett-Wilks - Bordoni relaxation), double intermediate-temperature (Hasiguti relaxation) and double high-temperature (the Ke-Mash-Hall grain-boundary relaxation) correlated peaks in internal friction, recrystallization peaks in nanostructured crystals (NSC) [2] and the macroscopic recrystallization in NSC. It is worth stressing that the same temperature dependences of activation energies and the mechanisms of all these processes [2] are in line with our data and confirm the universality of the above mechanisms in plasticity of solids [1].

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Plastic deformation mechanisms of MAX phase Ti_4AlN_3 and the core structure of dislocations

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Since their discovery in the late sixties, the MAX phases are subjected to tremendous studies because of their unique properties, combining the best of metals and ceramics. From the mechanical viewpoint, they are generally brittle at low temperature. The deformation mode is attributed to a dislocation-based model involving kink and shear bands and delamination.

Recently, an extensive analysis of as-grown Ti_4AlN_3 phase microstructure evidenced that contrarily to what is usually postulated in literature, the stacking faults associated to TiN intercalation in the structure possess an in-plane shear component [A. Joulain, L. Thilly and J. Rabier, *Phil. Mag.*, 88 (2008) 1307]. This new element implies to reconsider the role of planar defects in the plastic deformation. Indeed, this shear component can result also from the dissociation of dislocations promoting precipitation and a change in composition at the dislocation core when diffusion is available. This picture is analogous to what was found in YBCO superconductors [J. Rabier, P.D. Tall, M-F. Denanot, *Phil. Mag. A*, 67 (1993) 1021], where such “non stoichiometric” dislocations have been found to allow for stress relaxation in YBCO [A. Proult, P. D. Tall, J. Rabier, *J. Mater. Sci.* **36** (2001) 2451]. At high temperature where diffusion is more efficient the contribution of such defect to plasticity is likely to be important.

In this context, polycrystalline Ti_4AlN_3 has been plastically deformed at room temperature in order to prevent any diffusion onto the dislocation cores. To avoid cracks formation during compression tests at such a low temperature, a uniaxial stress has been applied under gaseous hydrostatic pressure using a Paterson press. The deformed microstructures have been analysed by transmission electron microscopy before and after in-situ annealing in order to investigate the role of diffusion on the dislocation core. The results are discussed in the context of the plastic deformation mechanisms relevant to MAX phases.

Deformation of anodic aluminum oxide nano-honeycombs during nanoindentation

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Anodic aluminum oxide with a nano-honeycomb structure is subjected to nanoindentation along the axial direction of the honeycomb. The load-displacement behavior is jumpy with periodic strain excursions. Top-view and cross-sectional microscopic examination reveals a very localized, “all-or-none” mode of deformation, with very clear-cut elasto-plastic boundaries. A crack system which is self similar with respect to the indent size is also found, and this is thought to correspond to the jumpy load-displacement behavior. A simple column model is proposed to explain certain features of the deformation microstructure.

Compressive deformation of tungsten coated aluminium micro-pillars

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Recent compression experiments on metallic micro-pillars revealed that their deformation is in general jerky with a stochastic nature [1-5]. The jerky nature of deformation implies that precise metal forming would be difficult in the micron regime. Two important features of the plasticity of micro-crystals have been suggested to be the nucleation [6,7] and annihilation [3,5] of dislocations at free surfaces. Suppression of these two mechanisms may alleviate the problem of jerky deformation, and this may be achievable by coating the pillars. In the present study, focussed-ion beam (FIB) milling was first used to fabricate micron-sized aluminium columns within a large grain. Their lateral surfaces were then coated by tungsten deposition using FIB, and the coated columns were then subjected to uniaxial compression by a flat-punch nanoindenter. In contrast to uncoated pillars, the coated columns showed smooth deformation, as is similar to a previous report of coated Au pillars [8]. A composite model also revealed that the coating significantly raised the strength of the core aluminium metal. Post-mortem TEM examination revealed that the dislocation density in the coated pillars increased significantly with the formation of tiny cellular structures after deformation. This is in sharp contrast to the behaviour of uncoated pillars, in which the dislocation density did not rise by more than an order of magnitude, and cells did not form after deformation [5]. The present study suggests that a thin coating can smoothen the deformation of micro-crystals, as well as strengthen them.

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Use of focused ion beam for investigating the mechanical properties of biological tissues: a study of human primary molar

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In this paper, the usefulness of the specimen shaping ability of focused ion beam (FIB) milling in the micron scale and the high force resolution of the nanoindentation technique are demonstrated on human primary teeth. Micro-cantilevers, with a triangular cross-section 5 μm in width and 10 μm in length, were produced within 50 μm of the amelo-dentinal junction (ADJ) using FIB milling, and were point-loaded at their free ends at 20 N/s until failure using a nanoindenter. The elastic modulus and failure strength of such micro-samples of human enamel, and their variation with respect to prism orientation, were studied and compared to data from bulk enamel measured using nanoindentation and three-point bend tests. The elastic modulus of the micro-cantilever samples was found to be comparable to that obtained by nanoindentation on bulk samples, but it demonstrates significant anisotropy commensurate with the microstructure of enamel which is not measurable using nanoindentation on bulk samples. The flexural strength of the enamel micro-cantilevers also exhibited strong anisotropy, and was about one order of magnitude higher than that of bulk specimens measured by three-point bending. Through a Weibull analysis, this size dependence of strength was found to be similar to the normal behaviour in brittle materials. The flexural strength of the enamel samples was also found to be sensitive to changes in the degree of mineralization of the samples.

Investigation of dislocation pile-up effects at grain boundaries by sub-granular indentation

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Grain-boundary (GB) strengthening is long thought to be due to the ability of a GB to stop dislocations, and to cause the well-known Hall-Petch effect of strengthening. In Petch's proposal (Petch 1953), propagation of slip to the next grain occurs when the stress concentration ahead of a dislocation pile-up at a GB triggers a source in the next grain to operate. The resistance of the GB to slip transmission in this mechanism is expressible by a critical stress intensity factor K_c , which depends on the misorientation across the GB and the source strength. The truth of the Petch mechanism, however, has never been verified directly. This project made use of nanoindentation to study the transmission of plasticity across GBs, by performing nanoindentation on one side of a GB, and seeing how slip was propagated to the other side. Experiments were carried out on two metallic materials with strong Hall-Petch effects: i) undoped Ni_3Al , and ii) niobium. In Nb, a second pop-in, in addition to the first pop-in due to incipient plasticity, occurred when indents were made near a grain boundary. The load at which this second pop-in occurred was approximately proportional to the square of the distance of the indent from the grain boundary. This observation is in agreement with Petch's concept of a critical K_c , and analysis using Johnson's cavity model of the indentation stress field could provide estimates of the K_c which are in good agreement with the macroscopically observed Hall-Petch slope for polycrystalline Nb. In Ni_3Al , no second pop-in related to grain boundary yielding could be observed, but scanning electron microscopy revealed clear evidence of intergranular slip transmission when the slip-system alignment across the grain boundary, quantified by a parameter m' , is low.