

Accelerated Multiscale Simulations of Incipient Plasticity using Hyper-QC

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The quasicontinuum (QC) method is a spatial multiscale method that extends the length scales accessible to fully-atomistic simulations (like molecular dynamics (MD)) by several orders of magnitude. While the recent development of the so-called "hot-QC method" [1] enables dynamic simulations at finite temperature, the times accessible to these simulations remain limited to the sub-microsecond time scale due to the small time step required for stability of the numerical integration. To address this limitation, we develop a novel finite-temperature QC method that can treat much longer time scales by coupling the hot-QC method with hyperdynamics – a method for accelerating time in MD simulations. We refer to the new approach as "hyper-QC" [2]. The temporal acceleration makes it possible to perform multiscale hot-QC simulations at near experimental loading rates for problems such as nanoindentation. An interesting observation regarding the possibility of entropically stabilized dislocations [3], uncovered in a hyper-QC simulation, will also be discussed.

[1] E. B. Tadmor, F. Legoll, W. K. Kim, L. M. Dupuy, and R. E. Miller, "Finite-Temperature Quasicontinuum", *Appl. Mech. Rev.*, **65**, 010803 (2013).

[2] W. K. Kim, M. Luskin, D. Perez, A. Voter, and E. B. Tadmor, "Hyper-QC: An Accelerated Finite-Temperature Quasicontinuum Method using Hyperdynamics", *J. Mech. Phys. Solids*, **63**, 94-112 (2014).

[3] W. K. Kim and E. B. Tadmor, Entropically Stabilized Dislocations, *Phys. Rev. Lett.*, in press (2014).

Molecular Dynamics Simulation Study of the Effect of Temperature and Grain Size on the Deformation Behavior of Poly-crystalline Cementite

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Molecular dynamics simulations combined with quantitative atomic displacement analyses were performed to study the deformation behaviors of poly-crystalline cementite (Fe_3C). At low temperature and large grain size, dislocation glide acts as the preferred deformation mechanism over grain boundary sliding. Due to the limited number of slip systems at low temperature, poly-crystalline cementite breaks by forming voids at grain boundaries upon tensile loading. When temperature rises or grain size reduces, grain boundary sliding becomes the primary mechanism and plastic deformation is accommodated effectively. Our observation sheds light on the origin of brittle-to-ductile transition in recently fabricated bulk sintered poly-crystalline cementite [1].

[1] M. Umemoto, Y. Todaka, T. Takahashi, P. Li, R. Tokumiya, K. Tsuchiya, Mater. Sci. Eng. A375-377 (2004) 894.

Fast Fourier Transform based Multi-scale Probabilistic Model of Twinning in HCP Materials

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Deformation twinning is an important deformation mechanism in hexagonal close packed (HCP) materials. It is a multi-scale process that depends on microstructural and mechanical responses at the meso, micro and atomic scales. Deformation twinning can be considered as a sequential process of nucleation followed by propagation and growth. The latter processes are responsible for hardening and texture evolution in HCP materials. In this work we focus on the stresses that are associated with the deformation twinning process. A full-field Fast Fourier Transform (FFT) based elasto-visco plastic formulation is modified to model probabilistic twin nucleation followed by propagation and growth in HCP materials. The local stresses at and in the vicinity of twins are quantified during twin nucleation, propagation and growth. An Mg polycrystal is used as the paradigm for implementing this approach. The findings and understanding from this work are translated to the more computationally efficient mean field models, such as self-consistent models.

Mechanical properties of nano-pillars containing a single homo- or heterogeneous interface

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Numerous studies on deformation of sub-micron, single-crystalline pillars have furthered our understanding of confined plasticity dominated by a free surface revealing a ubiquitous size effect. While this is of fundamental importance, most structural materials contain interfaces, such as grain boundaries in homogeneous polycrystalline structures or heterophase interfaces in multi-phase systems, which have important effects on their mechanical properties and can serve as sites for damage initiation. The behavior of lattice defects during post-elastic straining in such materials is thus complicated by the influence of boundaries.

We present experimental and computational results of the influence of a single high-angle grain boundary whose plane normal was inclined at an angle to the loading direction within individual Al nano-pillars subjected to uni-axial compression. We discuss their deformation in the framework of stochastic stress-strain signature indicative of nucleation controlled plasticity, as also revealed by molecular dynamics simulations and post-mortem TEM analysis. We also present experimental and computational results of uni-axial tension of nanopillars containing a single Fe/Fe-W metallic glass heterophase interfaces and explore the effect of interface morphology on their mechanical behavior. We employ molecular dynamics simulations to investigate the atomistic processes occurring at the interface and within the pillar bulk that govern deformation.

Scaling laws in the ductile fracture of metals

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Ductile fracture is the process whereby a material separates across a failure surface through mechanisms, such as void nucleation, growth and coalescence, which entail large amounts of plastic work. Owing to its engineering importance, ductile fracture has been the focus of extensive study since the 60's and one of the main driving forces in the development of nonlinear fracture mechanics. Unlike brittle fracture, where the behavior of the material is ostensibly elastic up to fracture, in ductile fracture the plastic dissipation attendant to void growth and coalescence accounts for a significant—or even dominant—part of the energy budget. Such extensive plastic deformation notwithstanding, failure ultimately takes place by separation across a plane or surface and entails a well-characterized amount of energy per unit area, or specific fracture energy, to operate. In consequence, typical measured specific fracture energies for ductile fracture are much larger than those of brittle solids and exhibit a characteristic temperature dependence that includes a brittle-to-ductile transition at a critical temperature. Recently, Fokoua *et al.* (2014) have performed a continuum optimal-scaling analysis of ductile fracture in metals and have shown that ductile fracture in metals can be explained as the outcome of two competing effects: their relatively low plastic-hardening rates, which enables geometric instabilities such as the necking and strain localization, and strain-gradient plasticity. The essence of their void-sheet construction may be understood as follows. Consider a slab of material of dimensions $L \times L \times H$, where H is the thickness of the slab. The slab deforms under periodic boundary conditions on its side and the other two faces of the slab are given displacements $\pm\delta$. Localize the deformations to a band of thickness a , and we subdivide this band into $\frac{L^2}{a^2}$ cubes of size a . We assume that the outside of the band moves rigidly, so that each cube deforms under periodic boundary conditions on its side with its other two faces displacing by $\pm\delta$. For large δ , we expect a void to nucleate from the center of the cube and the total energy of the voided slab/cube to scale as $E_{slab}^{tot} = \frac{L^2}{a^2} E_{cube}^{tot} = KL^2 \left[\left(\frac{\delta}{a}\right)^n a + l \frac{\delta}{a} \right]$ where K is a material constant, $0 < n < 1$ is the hardening exponent of the metal and $l > 0$ is the characteristic length of strain-gradient plasticity. The first term is due to plastic deformation as the void expands and the second term is due to the increase in surface area. Minimizing E_{slab}^{tot} with respect to a we obtain $a = \delta^\alpha l^{1-\alpha}$, with $\alpha = (1-n)/(2-n)$. Inserting these optimal values into the slab energy gives $E_{slab}^{tot} = KL^2 l^\alpha \delta^{1-\alpha}$, independently of the slab thickness H . In the present work, we carry out a similar analysis at the atomistic level. In so doing we explore whether the continuum scaling behavior extends down to the atomistic level, thus bypassing the need to model strain-gradient plasticity at the continuum level. We use an embedded atom method (EAM) model of Ni that reproduces the elastic and surface properties of Ni reasonably well. The calculations are performed with small orthorhombic single crystal unit cells of size $\sim 7.5 \text{ \AA} \times \sim 8.6 \text{ \AA} \times \sim 6 \text{ \AA}$ and direction $x=[1-10]$, $y=[11-2]$, $z=[111]$, which we scale by $2 < a/a_0 < 14$ in each direction, where a_0 is the cell size in the direction of deformation z . A void nucleus of 13 atoms is placed in each cell before deformation of $\pm\delta$ as above. The 3D periodic cell is relaxed to a minimum using standard molecular statics techniques. The cell energy as a function of a has a distinct minimum (sometimes multiple minima) for $0.25 < \delta/a_0 < 1$. Void growth and dislocation emission are clearly evident in the calculations. The cell scaling at the minimum cell energy has a linear logarithmic derivative $\alpha=0.58$ while the energy similarly scales with δ with $\alpha=0.68$. It is encouraging that the scaling of the cell size and energy are nearly consistent, but the value of $\alpha > 0.5$ implies the hardening exponent of nickel $n < 1$, which is clearly unphysical.

Increasing grain boundary cohesion to improve ductility of bcc transition metals

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The properties of grain boundaries (GB)s are of strong relevance for plastic deformation of bcc refractory metals. In fact, brittle crack advance and ductile deformation are two simultaneous and competing processes for which the cohesion of the GBs plays a central role. Molybdenum and tungsten are two metals which exhibit low GB cohesion resulting in a high ductile-to-brittle-transition temperature (DBTT) low toughness and intergranular fracture. In order to lower the DBTT and in this way improve the mechanical properties, it is essential to develop a thorough understanding of the interplay between GB geometry, the segregation of solute elements to the interface and the work of separation.

We present atomistic simulations of GBs in tungsten, molybdenum and ferritic iron. Our approach is based on density-functional theory and the embedded atom method to efficiently obtain reliable GB geometries. We scan over a wide range of GBs, selecting those, which are highly frequent in real polycrystals, and investigating the change of properties (i.e. the geometry, work of separation, GB energy) as a function of misorientation. In this way we provide a comprehensive overview of GB cohesion for pure bcc metals in an unprecedented quality. Furthermore, the segregation of a number of solutes to the GB and the surface and their effect on GB cohesion for Mo and W is studied. Herein we present a new approach which combines the traditional method for studying solute segregation in the highly dilute limit with a first-principle mean field approximation (the virtual crystal approximation) to investigate segregation in highly alloyed metals. We discuss the correlation between segregation and GB cohesion and the implications arising for the DBTT temperature.

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Size Dependent Strength of Nanoparticles – A Combined Experimental/Computational Study

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It is well established that materials can drastically change mechanical properties when their size is reduced to the nanoscale, mainly because of an increase in surface to volume ratio and of lowering the amount of defects in the lattice. Recently, we suggested employing nanoparticles as specimens to study strength at the nanoscale [1,2]. An ensemble of faceted, single-crystal, mobile-dislocation free nanoparticles is produced on a sapphire substrate via dewetting of thin-films. The nanoparticles were indented with a sharp tip or deformed under compression. In this talk, we show how the combination

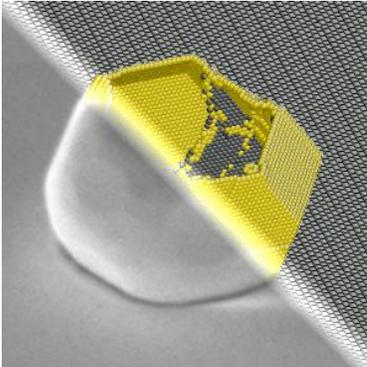


Figure 1: A reproduction of a gold nanoparticle from a SEM image and a molecular dynamics simulation.

between the experimental results and atomically-informed dislocation mechanisms allows us to study mechanical properties at the nanoscale. An indentation size effect is observed experimentally, which is rationalized with molecular dynamics (MD) simulations as the competition between dislocation storage and depletion on free surfaces. Moreover, the dependence of their yield stress under compression on their size can be described by a power law. From both MD simulations and finite elements analysis we conclude that the yield point is dislocation nucleated-controlled and we propose a model to rationalize the power-law dependency. We discuss how the mechanical response of the nanoparticles to compression and indentation depends on material properties and crystal structure,

which manifests itself through the underlying dislocation mechanism.

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Linking Atomistic, kinetic Monte Carlo and Crystal Plasticity simulations of single-crystal Tungsten strength

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We present a multiscale model that comprises atomistics, kinetic Monte Carlo and continuum-level crystal plasticity calculations, to simulate the plastic response of tungsten crystals in uniaxial tension tests. Molecular statics calculations are used (i) to study the energetics of kink-pair nucleation as a function of stress for screw dislocation motion, and (ii) to obtain the critical stress deviation from Schmid's law. The atomistic data are used to parameterize a kinetic Monte Carlo model used to simulate thermally-activated screw dislocation motion and to obtain the mobility laws on different slip planes. The dislocation mobility laws obtained from the kMC model are embedded as constitutive law into a dislocation-based crystal plasticity framework, which is used to perform material point simulations and compute the yield strength in single crystal tungsten under different uniaxial loading orientations of the standard triangle.

Modelling Mechanical Behaviour of Quantum Solids using Path-integral Monte Carlo Simulations

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The mechanical behavior of quantum crystals, in which the magnitude of the zero-point kinetic energy is appreciable compared to the energy scale of the interatomic interactions, has become a topic of increasing interest. A system that has received particularly significant attention is crystalline ⁴He, the prototypical bosonic quantum crystal. After initial indications of superfluidity in this crystal [1], extensive experimental effort has been directed toward the mechanical properties of this system. Indeed, observations of elastic stiffening have been linked to dislocation behaviour and the role of isotopic ³He impurities [2,3].

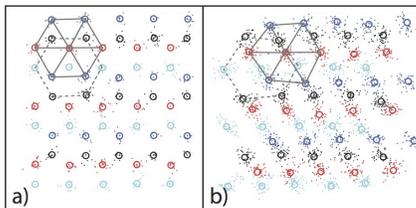


Figure 1: PIMC simulation of homogeneous stacking-fault nucleation in hcp ⁴He under homogeneous shear deformation.

Despite an extensive body of experimental data [4], their interpretation has systematically relied on assumptions concerning the involved fundamental materials parameters, which are inaccessible experimentally. Here, we show how fully atomistic path-integral Monte Carlo (PIMC) simulations [5] can be used to compute such parameters and provide insight into the basic deformation mechanisms involved in systems dominated by quantum effects.

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