Stress Dependence of the Peierls Barrier in BCC Metals

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The Peierls barrier of a dislocation is defined as the dependence of the energy of a dislocation on its position along a path between two crystallographically equivalent locations of the dislocation. The Peierls stress is then the stress necessary to surmount this barrier at 0 K and it is related to the maximum derivative of the barrier with respect to the dislocation position. In majority of studies the Peierls barrier has been considered as fixed, determined by the crystal structure and corresponding interatomic interactions in a given material. This implies that the same should apply to the Peierls stress. Nonetheless, recent atomistic studies of ½<111> screw dislocations in transition BCC metals have shown that their Peierls stress is strongly dependent on the applied stress tensor, in particular on shear stresses parallel and perpendicular to the Burgers vector. This implies that the Peierls barrier also depends on the applied stress tensor in asimilar way. However, while the Peierls stress is readily obtained in atomistic calculations, the corresponding Peierls barrier cannot be directly determined. In this paper we show how the stress-dependent Peierls barrier can be ascertained from the atomistic data of the stress dependence of the Peierls stress. This is done by introducing the Peierls potential that is a function of two coordinates that represent the position of the intersection of the dislocation line with the {111} plane perpendicular to the corresponding <111> slip direction. The Peierls barrier is then sought as the lowest energy path over the two-dimensional Peierls potential. This potential that is then self-consistently adjusted such as to reproduce the stress-dependence of the Peierls stress. This procedure is tested using the nudge-elastic-band model to determine the Peierls barrier in a given material without introducing first the Peierls potential. Finally, it is shown that when employing this barrier in the model of the formation of kink-pairs at finite temperatures the observed orientation dependences of the yield stress in molybdenum are well reproduced.

Dislocation Dynamics in Metals at Atomic-scale:

I. Interactions between Dislocations and Obstacles with Dislocation Character

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Irradiation of metals with high-energy atomic particles creates nano-scale defect clusters. This presentation will be concerned with those that have dislocation character, i.e. dislocation loops and stacking-fault tetrahedra. Depending on the reactions involved, they can act as obstacles to dislocation glide during plastic flow and can give rise to hardening and, in some conditions, strain localisation. Treatment of these effects in the elasticity theory of dislocations is problematic without information about the atomic-scale mechanisms that occur during dislocation-obstacle interaction. Computer simulation can provide details of the influence of stress, strain rate and temperature on the mechanisms, and thereby on the consequent obstacle strength and possible changes in the irradiation microstructure. Simulations of static conditions (temperature = 0K) provide for direct comparison with results from the continuum treatment of dislocations. Recent results for dislocations gliding under stress against obstacles in a variety of metals across a range of temperature are classified in this presentation. The effects observed vary from reactions in which the dislocation and obstacle are left unchanged, through ones in which the obstacle is changed but the dislocation is not, to ones in which the obstacle is absorbed temporarily or permanently by the dislocation. Despite the small length scales involved, products of the reactions can be understood within the continuum approximation in many cases.

A recent comprehensive review of atomic-scale computer simulation of dislocation-obstacle interactions is to be found in:
D.J. Bacon, Yu.N. Osetsky and D. Rodney, 'Dislocation-obstacle interactions at the atomic level', in Dislocations in Solids, eds. J.P Hirth and L. Kubin, vol. 15, Elsevier, 2009, chap. 88, pages 1-90.

Dislocation Dynamics in Metals at Atomic-scale:

II. Interactions between Dislocations and Obstacles with Inclusion Properties

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Irradiation of metals with high-energy atomic particles creates nano-scale defect clusters. In addition to those with dislocation character described in part I, three-dimensional defects, such as voids, gas-filled bubbles and secondary phase precipitates, may form. Rigid oxide particles are also important microstructure features of oxide-dispersion-strengthened (ODS) materials. In terms of the resistance they provide to dislocation glide, these inclusion-like clusters provide a variety of mechanisms, ranging from simple shear to structural transformation to impenetrability. We present atomic-scale modelling of an edge dislocation in Fe interacting with such obstacles, with the aim of identifying the mechanisms that control dislocation breakaway and understanding the conditions when maximum obstacle strengthening are realized. We demonstrate that screw dislocation cross-slip and associated climb of edge dislocations are important processes for decreasing effective strength of some obstacles. Conditions for achieving the maximum possible strength are discussed.

If time permits, recent modelling of nano-indentation using large-scale molecular dynamics will be reported. Mono-crystals of Fe and Cu with different indentation surfaces and Cu bi-crystals containing a twin boundary have been investigated using spherical and cylindrical indenters with radius up to 60nm. Generation of dislocations and dislocation loops was found to be dependent on the specimen type and surface, and indenter rate. A variety of mechanisms was observed, including reactions between mobile dislocation loops and dislocations in Fe and Cu, generation and unzipping of sessile configurations in Cu and transformations between different dislocation loops in Fe. It was also observed that a twin boundary in Cu is a strong obstacle for glissile dislocations and dislocation loops, and that it can act as a dislocation source after intensive interaction with glissile dislocations at large load.

Atomistic Mechanisms of Twin Boundary Motion in Temperature and Stress Fields

Nasr M. Ghoniem (UCLA), Lan Li (Microsoft), Anthony Brown (UCLA), Qiyang Hu (UCLA)

The migration kinetics of coherent twin boundaries (CTBs) and the underlying atomistic mechanisms are revealed through Molecular Dynamics (MD) computer simulations. Details of the motion dynamics and associated effective migration of CTBs are examined for nanotwinned copper crystals under externally applied shear loading. It is found that the dynamics of CTB motion can be described as a “stick-slip”process. The present study reveals that the magnitude and direction of the resulting CTB migration velocity is dependent on the shear-loading orientation. It is shown that (112)-type shearing of the twin boundary maximizes its transverse migration velocity. Shearing at directions which remain parallel the TB plane but are inclined to the (112)-direction results in gradual decoupling of the transverse and sliding motions, and finally to TB-sliding alone when the shear direction is along (110). Detailed analysis of atomic configurations indicates that the “stick”step of the dynamics is a result of accumulated strain in the crystal that is released by the nucleation of Shockley partial dislocation loops on the twin boundary. Dislocation nucleation is preceded by coordinated shuffling of atoms in atomic layers adjacent to the twin boundary. Initiation sites for nucleation events are observed at the atomic layer directly adjacent to the twin boundary, at the surface of the crystal, and at stress concentration regions associated with the motion of shuffled atoms in the crystal interior. The “slip”part of the dynamics is shown to be controlled by the fast propagation of nucleated Shockley partials and their spreading along the twin boundary.

Plasticity in Carbon Nanotubes: Cooperative Conservative Dislocation Motion

Shuo Chen, Elif Ertekin, Daryl C. Chrzan

Monte Carlo simulations are used to study dislocation glide mediated plasticity in carbon nanostructures. A detailed analysis of the simulations leads to identification of a new type of defect, a dislocation screened by multiple dislocaiton dipoles, as the mediator of plastic deformation. The defects appear under high stress conditions. The appearance of these defects is rationalized in terms of the competition between dislocation core energy and the buckling inherent to dislocation motion within an essentially two dimensional membrane. These defects thus represent a deformation mechanism that is uniquely found in nominally two-dimensional nanostructures. The influence of these defects on the predicted mechanical properties of carbon nanostructures is discussed.

Discrete dislocations in grapheme

Pilar Ariza and Michael Ortiz,
U. of Seviile, and Caltech

We present an application of the theory of discrete dislocations to the analysis of dislocations in graphene. We discuss the specialization of the theory to graphene and its further specialization to the force-constant model of Aizawa et al. (1990). The ability of the discrete dislocation theory to predict dislocation core structures and energies
is critically assessed for periodic arrangements of dipoles and quadrupoles. We show that, with the aid of the discrete Fourier transform, these problems are amenable to exact solution within the framework of discrete dislocation theory, which confers the theory a distinct advantage over conventional atomistic models. In particular, the discrete dislocation theory predicts 5-7 ring core structures that are consistent with observation and dislocation energies that fall within the range of prediction of other models.
The asymptotic behavior of dilute distributions of dislocations is characterized analytically in terms of a discrete prelogarithmic energy tensor. Explicit expressions for this prelogarithmic energy tensor are provided up to quadratures.

Driving Forces on Moving Defects: Dislocations and Inclusions

Xanthippi Markenscoff and Luqun Ni, UCSD

“Driving forces" on moving "defects are very important for the study of the evolution of "damage "zones etc. They are defined as configurational forces on the basis of the variation of the total (including external forces) Lagrangean of the system under infinitesimal transformations, which results in the “contour independent” dynamic J integral .Dislocations and inclusions are “defects” that possess self-stresses due to incompatibility of the deformation. For dislocations, the dynamic-self force (which results in an "effective mass" associated with accelerating the dislocation) is obtained for both subsonic and transition to supersonic motion. For an expanding Eshelby inclusion the radiated fields including inertia effects are obtained, and those of a half-space inclusion moving from rest in general subsonic motion are calculated by a limiting process from the spherically expanding inclusion (with dilatational eigenstrain) as the radius tends to infinity. The global energy-release rate (of the mechanical work),self-force-, required to move an inclusion boundary and to create an incremental region of eigenstrain is defined and obtained for a plane boundary under general eigenstrain , thus extending the energy-release rate and the dynamic J integral treatment already well established for dislocations and cracks to a defect that is a jump discontinuity. The equation of motion, based on the “Eshelby principle” of total driving force equal to zero, is obtained. It contains two terms, for dislocations as for inclusions: the self-force and the Peach-Koehler force due to an applied stress field.

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Markenscoff, X. and Ni, L. (2010) “The energy-release rate and self-force of dynamically expanding spherical and plane inclusion boundaries with dilatational eigenstrain”
J. Mech. Phys. Sol. 58, 1-11.

The Peierls stress for coupled partials near a free surface (variable core model)

Benoît Gars, Ecole Polytechnique, Paris and Xanthippi Markenscoff,
UC San Diego

The variable core dislocation model of Lubarda and Markenscoff (2006), which gives the Peierls-Nabarro one as special case, allows for the core radius to vary as the dislocation moves through the lattice. Here, the core interactions among two partials are modeled with good agreement with atomistic calculations, and the Peierls stress is obtained from this model. For a perfect dislocation, and dislocation partials near a free surface, the core radius is allowed to depend of the distance *h* from the surface, the energies are calculated as a function of them, and the Peierls stress is obtained as a function of *h*. It is also shown that the cores of the partials merge as the dislocations approach the free surface, in agreement with atomistic results in the literature.

1. Lubarda, V and Markenscoff, X. "A Variable Core Model and the Peierls Stress for the Mixed (Screw-Edge) Dislocation," Appl. Phys. Lett, 89, no. 151923, 2006.
2. Lubarda, V. and Markenscoff, X. "Configurational Force on the Lattice Dislocation and the Peierls Stress," Arch. Appl. Mech., 76, December 2006.

Size and Scale Effects in Crystal Plasticity

Amine Benzerga,
Texas A& M

Plastic deformation takes place in solids due to fine-scale microstructural rearrangements. In crystalline materials, the latter are mediated by the generation and motion of lattice defects called dislocations. There is an increasing amount of experimental evidence that the plastic behavior of crystals changes at micro- and nano-scales in a way that is not necessarily captured by state-of-the-art plasticity models. In this talk, I will analyze length scale effects in the plasticity of crystals by means of direct numerical simulations that resolve the scale of the carriers of plasticity, i.e., the dislocations themselves.
I will introduce a computationally efficient, atomistically informed dislocation dynamics framework which has the capability of reaching high dislocation densities and large strains at moderately low strain rates in finite volumes. I will then present our discovery of a new type of size effect in the hardening of crystals subject to nominally uniform compression. In an attempt to develop improved continuum models, I will present an analytic work targeted at characterization of structure, its evolution and resolution dependence. In light of such findings, I will discuss behavior transitions in the space of meaningful structural parameters, from forest-hardening dominated regime to an exhaustion hardening dominated regime. Various scalings of the flow stress with crystal size emerge in the simulations, which are compared with recent experimental data on micro- and nano-pillars.

High Velocity Dislocations

M. A. Meyers, UCSD
B. A. Remington, LLNL
E. M. Bringa, U. Nacional de Cuyo, Argentina
Y. Tang, UCSD

We are exploring shock compression of metals as a means to drive dislocations at high velocities. The shock front accelerates dislocations and, in the process, the deviatoric stresses are attenuated. Experimental results are compared with analyses and molecular dynamics simulations.
Reference:

Reference: M. A. Meyers, H. Jarmakani, E. M. Bringa, B. A. Remington, Dislocations in Shock Compression and Release, in "Dislocations in Solids," eds. J. P. Hirth and L. Kubin, Vol. 15, Elsevier, 2009

Atomic Level Calculations of Deformation in Small Structures

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and
University of California, San Diego

One of the classic problems in materials science is the hardening of metals. We know that dislocation-dislocation interactions are critical in explaining this phenomenon, but dislocation core effects dominate these interactions. Thus understanding of hardening must be obtained at the atomic level. Recently experiments have shown that the hardening of materials depends upon the size of the sample. One interpretation of these experiments is that the phenomenon is caused by strain gradients. Atomistic calculations in nickel using the Embedded Atom Method (EAM) will be presented that show a size effect of the yield stress is present in small single crystals of Ni under simple shear, an imposed strain state that does not have a gradient.

Compression experiments have been recently performed in small single crystal pillars of W. A number of EAM calculations have been performed to parallel these experiments. The results of these calculations will be presented, emphasizing the role of dislocations in small volumes.

Dislocation Dynamics in Sub-Micron Pillars under Compression and Torsion

Wei Cai
Mechanical Engineering Department, Stanford University

In single crystal metal micro-pillars under compression, the balance between the dislocation multiplication rate and exhaustion rate (at the surface) may be the key to understand the observed size effect in flow stress. Here we report two counterintuitive observations from Molecular Dynamics and Dislocation Dynamics simulations. In body-centered-cubic (BCC) metals, the surface itself is sufficient to induce dislocation multiplication as a single dislocation moves across the pillar. In face-centered-cubic (FCC) metal pillars and thin films, however, even jogs of the Lomer-Cottrell type are not strong enough pinning points to cause dislocation multiplication. These results highlight the need for better calibration of Dislocation Dynamics models against the more fundamental atomistic models.

In single crystal nanowires under torsion, we show that the deformation can be either homogeneous
or heterogeneous, regardless of size, depending on the wire orientation. Homogeneous deformation occurs when <110>-oriented face-centered-cubic metal wires are twisted, leading to the nucleation of co-axial dislocations, analogous to the Eshelby twist mechanism. Heterogeneous deformation is predicted for <111> and <100> wires under torsion, localized at the twist boundaries. These simulations also reveal the detailed mechanisms of twist boundary formation from dislocation reactions.

Ref:
[1] C. R. Weinberger and W. Cai, “Surface-controlled dislocation multiplication in metal micropillars”, Proc. Nat’l Acad. Sci. 105, 14204, 2008.

[2] C. R. Weinberger and W. Cai, “Orientation dependent plasticity in metal nanowires under torsion: twist boundary formation and Eshelby twist”, Nano Letters, in press (2010).

A Twist of the Eshelby Twist: A Pole Mechanism of Twinning for Sustainable Ultra-strength Deformation

Ting Zhu
Woodruff School of Mechanical Engineering, Georgia Institute of Technology

The principal difficulty in understanding the deformation mechanisms of small-volume crystalline solids has been to explain how the plastic deformation carriers such as dislocations and twins are generated and multiplied. The sources of such carriers have not been well established in small crystals with dislocation-limited characteristics. In 1953, Eshelby showed that the central region of a thin rod can act as a trap to stabilize the skew dislocation lying parallel to the axis of the rod, and the axial skew dislocation spontaneously induces the torsional deformation of the rod â^' the so-called Eshelby twist (Eshelby, J. Appl. Phys., 24, pp. 176, 1953). Such an axial screw, in addition to being central to crystal growth, can result in regenerative inelastic shear for continued plastic flow. This is achieved through a 3D process of dislocation intersection followed by a new pole mechanism of twinning, providing an efficient approach of realizing the sustainable deformation in nanomaterials with ultrahigh strength.

Role of the defect core in energetics of vacancies

Vikram Gavini,
U. of Michigan, Ann Arbor

This talk presents recent investigations into the crucial role of a defect-core in the energetics of vacancies in aluminum using electronic structure calculations at macroscopic scales [1,2]. We find that vacancy core-energy is significantly influenced by the state of deformation at the vacancy-core, especially volumetric strains. Insights from the core electronic structure and computed displacement fields show that this dependence on volumetric strains is closely related to the changing nature of the core-structure under volumetric deformations. These results are in sharp contrast to mechanics descriptions based on elastic interactions that often consider defect core-energies as an inconsequential constant. Upon studying the influence of various macroscopic deformations, which include volumetric, uniaxial, biaxial and shear deformations, on the formation energies of vacancies, we show that volumetric deformations play a dominant role in governing the energetics of these defects. Further, by plotting formation energies of vacancies and di-vacancies against the volumetric strain corresponding to any macroscopic deformation, we find that all variations in formation energies collapse on to a universal curve. Implications of these results in the context of dynamic failure in metals due to spalling are analyzed.

References:
[1] Role of macroscopic deformations in energetics of vacancies in aluminum, Phys. Rev. Lett. 101 205503 (2008).
[2] Role of the defect-core in energetics of vacanices, Proc. Roy. Soc. Lon. A 465 3239-3266 (2009).

A Multiscale Cohesive Zone Model and Simulations of Fractures

By Shaofan Li and Xiaowei Zeng
University of California at Berkeley

An atomistic based multiscale cohesive zone model has been proposed.
In this approach, coarse grain models are adopted both the bulk medium and the material interfaces, or defects. The material interfaces are considered as the weakest link in the model, the cohesive zone between two bulk media is remodeled as a finite width strip whose lattice constants and atomistic (depletion) potential are different from those of the bulk medium.
We use the Derjaguin's approximation to obtain the depletion potential inside the cohesive zone. That is: we assume that the cohesive zone is a compliance interface that is much weaker than the two adjacent bulk elements. The cohesive strength of the cohesive zone is determined by the van der Waals force or interactions between the cohesive zone and the bulk medium. Since we know the atomistic potential inside the bulk medium, we can obtain the depletion atomistic potential of the cohesive zone by integrate the bulk potential over the rigid bulk medium half space under assumption that the bulk medium is rigid with almost no deformation comparing to cohesive zone region.

Furthermore, we argue that the effective deformation gradient of the cohesive zone may be obtained based the FEM nodel displacements that are shared by the cohesive element. By doing so, we can use an effective Cauchy-Born rule to determine the effective stress and strain inside the cohesive zone so that the effective traction force along the bulk elements can be obtained.

The multiscale cohesive zone model has been applied to simulate crack propagations in both 2D and 3D cases in both single crystal as well as polycrystals. We have defined and discovered a so-called element mesh stacking fualt energy, whose behavior will result different fracture patterns such as brittle fracture as well as ductile fracture. Crack branching and void formation have been found all possible for different element mesh stacking fault energies which are dictated by the effective lattice structure or microstructure in the interface.

Dipole pile-ups and helical instabilities: Asymptotic methods in dislocation modelling

C L Hall with Y Zhu,
Oxford University,

The methods of asymptotic analysis can be applied to a wide variety of problems in dislocation modelling. In this talk, two distinct but related problems are presented in which asymptotic methods are useful. Firstly, we look at the interaction of a large number of edge dislocation dipoles. By appropriately defining a dipole density function, it is possible to contruct a differential equation for dipole density that is analogous to the singular integral equation for dislocation monopole density in a conventional pile-up. Interestingly, boundary layers arise in which the dipoles must be considered discretely. Secondly, we present findings on helical instabilities of a single dislocation that is very close to being a screw dislocation. Most dislocation mobility laws restrict the motion of a dislocation with edge component to its glide plane. However, by considering a mobility law where dislocation segments that are almost screw can slip out of their glide-plane, it is possible to show that straight dislocations with a small edge component exhibit helical instabilities.

[References: we have one submitted paper that is relevant to the first half, but most of this work is still being written up.]

Stress induced inhomogeneous destabilization mechanisms in ideal crystals

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The presentation will focus on the following topics: the theory of crystal stability and bifurcation under load [1-3], lattice statics [3-7] and molecular dynamics [8-12] studies of the mechanisms for destabilization of crystals under load at the limits of elastic stability, and questions such as whether lattice destabilization will lead to a phase transformation or fracture [7, 8, 12]. As an example, molecular-dynamics simulations of a bcc metal under <100> uniaxial load reveal a new fundamental understanding of the atomistic kinematics and dynamics of the stress induced crystallographic transition from the body centered cubic to the hexagonal close packed structure [12]. The transformation occurs with opposing shearing of alternate {110} planes; however, shearing occurs on the {110} planes of zero shear stress, contrary to what would be expected from classical plasticity theory. The results, including the singular nature of the lattice parameter variations at the inception of the transition, are analyzed and explained within the framework of crystal elastic stability theory.

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8. “Atomic Pattern Formation at the Onset of Stress-Induced Elastic Instability: Fracture versus Phase Change,” F. Milstein, J. Zhao, and D. Maroudas, Phys. Rev. B, Vol. 70, pp. 1841102 (2004).
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12. “Dynamics of the bcc-hcp transition in crystals under uniaxial stress,” H. Djohari, F. Milstein, and D. Maroudas, Phys. Rev. B, Vol. 79, 174109 (2009).