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6. AUTHOR(S)
L.B. Freund, Prof. of Engineering
M. Ortiz, Prof. of Engineering
R. Phillips, Prof. of Engineering

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Brown University
Division of Engineering
182 Hope Street
Providence, RI 02912

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Deformation processes in crystalline materials of engineering significance are considered which are beyond the reach or atomistic simulations, due to the need to consider practically significant volumes of material, and beyond the reach of continuum mechanics, due to need to consider physical aspects of material defects. This work is based on a method of spatial discretization well-suited to multiple-scale analysis and the explicit consideration of the lattice geometry in the reference consideration of the crystal. Computational strategies have been developed which (i) include stable lattice defects (dislocations) in the solution (ii) yield an unambiguous value for dislocation core energy, (iii) agree with atomistic theory over those small regions where they can be compared, and (iv) produce an approach to integration of crystalline defect physics into continuum analysis which is currently being pursued for several applications. In addition, a continuum study of dislocation nucleation at the surface of a highly stressed solid has been pursued which takes into account the core structure of the dislocation. While the activation energy for this process estimated on the basis of dislocations without core features is unrealistically large, it is found that the inclusion of core structure brings the activation energy estimates into the range of physically realizable behavior.

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BROWN UNIVERSITY Providence, Rhode Island 02912
Division of Engineering
Box D
Fax (401) 863-1157

March 7, 1995

To: Dr. Walter F. Jones, Program Manager, Directorate of Aerospace Sciences, Air Force Office of Scientific Research

From: L. B. Freund, M. Ortiz and R. Phillips, Division of Engineering

Re: Final Technical Report, Grant No. F49620-92-J-0129

This memorandum is a summary report of research on this grant during the period from 1 January 1992 through 31 December 1994. We are pleased to report that the principal objectives have been met, and that directions for advance at the continuum/atomistic interface have been defined in the course of this work. Through incorporation of the perspectives from several disciplines normally regarded as disjoint, we have extended concepts of mechanics beyond traditional boundaries and have identified fruitful avenues for research in the area of mechanics of materials.

Finite element analysis of inelastic processes

The analysis of the core structure of crystal defects such as dislocations, vacancies and solute atoms requires consideration of anharmonic lattice effects near the core. Lattice statics or molecular dynamics based on atomistic energy functions provide a powerful and accurate analysis tool on this scale. At the other end of the spectrum the macroscopic deformation behavior of crystals may involve dislocation densities as high as 10^{15} m^{-2}. An area of one mm^2, e. g., near the tip of a crack, may be crossed by as many as 10^9 dislocations. This precludes consideration of individual dislocations at the macroscopic scale, and has spurred the development of constitutive models which treat dislocations and other defects as continuously distributed objects. An intermediate scale, on the order of a few hundred nm, is presently emerging as the focus of increasing attention in applications such as nanoindentation. This scale is presently beyond the reach of atomistic methods. However, the deformation processes of interest involve discrete dislocations in numbers which are too small to be adequately described by macroscopic crystal plasticity models. This is the scale which we preferentially address in the present work.

Ideally, we would like to have **one** theory with the following attributes. At the *macroscale*, the theory should reduce to continuum crystal elasticity, with its usual properties of material frame indifference and crystal symmetry. At the *microscale*, the theory should be built upon an atomistic potential, incorporate a lattice parameter, and possess all the usual lattice invariance properties. We note that the incorporation of the lattice parameter as an intrinsic length necessarily renders the theory nonlocal. At intermediate or *mesoscales*, the theory should exhibit a continuous or

seamless transition from the lattice to the continuum realms.

One way in which such a theory can be constructed is as follows. We begin by considering an equilibrated reference composite Bravais lattice $\mathbf{X}(\mathbf{l},k)$, $\mathbf{l}\in Z^3$, $k=1,\ldots,s$. We adopt the Cauchy-Born rule and assume that, locally, deformations are affine, possibly with shuffles. Consequently, the positions of the atoms in the deformed configuration are

$$\mathbf{x}(\mathbf{l},k)=\mathbf{F}\mathbf{X}(\mathbf{l},k)+\mathbf{b}(k),\qquad \mathbf{l}\in Z^3,\ k=1,\ldots,s \tag{1}$$

where $\mathbf{F}$ is the local deformation gradient. The strain energy density of the crystal follows as

$$W(\mathbf{F})=\lim_{V\to\infty}\frac{1}{V}\min_{\mathbf{b}(k)}\Phi\big(\mathbf{x}(\mathbf{l},k)\big) \tag{2}$$

where Φ is some atomistic potential. Note that the shuffles are optimized locally for given $\mathbf{F}$. The use of an atomistic potential and the Cauchy-Born rule, and the explicit consideration of the lattice geometry in the reference configuration of the crystal, automatically endows the energy density function with the following properties: i) material frame indifference, $W(\mathbf{QF})=W(\mathbf{F})$, $\forall\mathbf{Q}\in \mathrm{SO}(3)$; ii) crystal symmetry, $W(\mathbf{FQ})=W(\mathbf{F})$, $\forall\mathbf{Q}\in\mathcal{S}$ where $\mathcal{S}$ is the point symmetry group of the lattice; iii) lattice invariance, $W(\mathbf{FH})=W(\mathbf{F})$, $\mathbf{H}\in Z^{3\times 3}$, $\det\mathbf{H}=\pm 1$; iv) slip-invariance, $\mathbf{H}=\mathbf{I}+\gamma\mathbf{c}\otimes\mathbf{b}$, $\mathbf{c},\mathbf{b}\in Z^3$, $\mathbf{c}\cdot\mathbf{b}=0\Rightarrow W(\mathbf{H})$ periodic in γ with period 1.

Stable configurations of the crystal can now be identified with minimizers of the potential energy

$$P[\phi]=\int_{B_0}W(\mathbf{F})dV_0-\text{forcing terms} \tag{3}$$

where B_0 is the domain of the reference configuration of the crystal, $\phi: B_0\to R^3$ is the deformation mapping, and the attendant deformation gradients follow as $\mathbf{F}=\nabla_0\phi$. Evidently, for small deformations of the crystal, the formulation reduces to conventional anisotropic linear elasticity. In particular, energy minimizers are uniquely defined up to a rigid body motion. These conditions are commonly realized in regions of the crystal which are distant from lattice defects. However, property (iv) implies the lack of quasi-convexity of W [1], which in turn makes it possible for energy minimizers to develop intricate microstructures on a fine scale, such as lattice defects, twinning and others. On this scale, the periodicity of the lattice, and the resulting periodicity of the energy function with respect to crystallographic slip become all-important.

For reasons which will become apparent in the sequel, an **essential** building block of the present approach is the introduction of a method of spatial discretization well-suited to multiple-scale analysis. Adaptive finite elements constitute a prime example. In our work, we have followed the approach of Ortiz and Quigley [2]. The reference domain of the crystal B_0 is partitioned into N six-noded triangular elements Ω_h^e, $e=1,\ldots,N$. Here and subsequently, the subscript h refers to some measure of the finite element mesh size. The deformation mapping ϕ_h is interpolated from nodal values using quadratic shape functions. Integrals over the elements, such as required for the computation of the energy, are approximated by a three-point quadrature rule. The stresses and tangent moduli are computed from the atomistic potential at the quadrature points of the elements based on the local value of the deformation gradients. The nodal values of the interpolated deformation mapping ϕ_h are obtained by a conjugate gradient iteration with line searches.

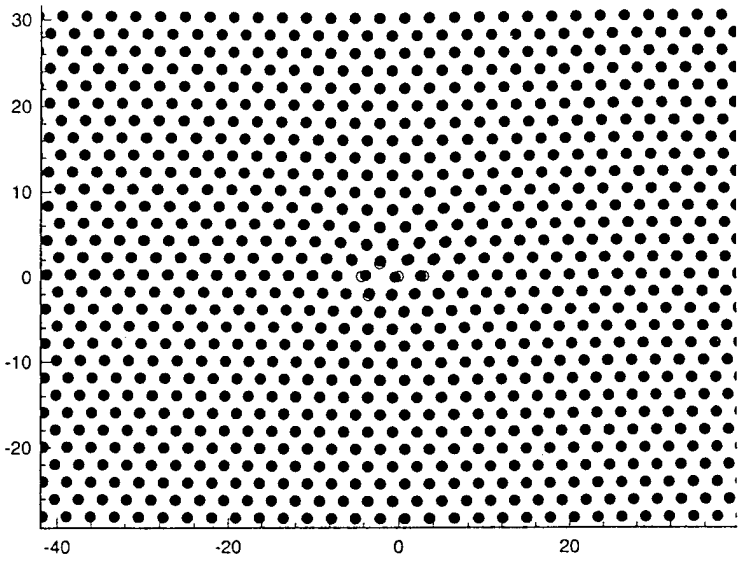

Fig. 1. Comparison of core structures of a Lomer dislocation in aluminum as computed by quasi-continuum method (black) and a direct atomistic simulation (grey).

Meshes are constructed by Delaunay triangulation based on the corner nodes of the elements. Elements whose strain energy exceeds a specified maximum, i. e., such that

$$\int_{\Omega_h^e} W(\mathbf{F}_h) dV_0 > TOL \tag{4}$$

are targeted for refinement. This adaption criterion results in equipartition of energy over the elements of the mesh. Elements are refined by introducing new corner nodes at midside locations, followed by a complete re-triangulation of the mesh. The nodal displacements and state data are transferred to the new mesh using a transfer operator derived by Ortiz and Quigley [2].

It should be carefully noted that the theory, as previously stated, is purely local, as it lacks a characteristic length scale. This is a consequence of the adoption of the Cauchy-Born rule, which renders the energy density independent of the lattice parameter a. Minimizers of local energy functions lacking quasi-convexity often develop structure at arbitrarily fine scales. In particular, the energy equipartition criterion leads to indefinite mesh refinement near the core of defects such as dislocations. The requisite physical cut-off is, evidently, the lattice parameter a. We therefore endeavor to restore the lattice parameter a into the theory.

This can be accomplished by a variety of means. Some possibilities are strain-gradient theories and non-local theories of the integral type, to mention a salient few. The common feature of these formulations is that they filter out the short wavelength components of the Fourier transform of the deformation gradient field. But in the context of adaptive finite element calculations, the same identical effect may be expediently accomplished by limiting the **spatial resolution** of the mesh, i. e., by requiring

$$h \geq h_{\min} \sim a \tag{5}$$

In this manner the lattice parameter a is restored into the theory as an intrinsic length.

The introduction of a mesh-size cut-off effectively checks the process of indefinite refinement induced at the core of defects by the energy equipartition adaption criterion. This in turn results in well-defined core energies, a prime distinguishing characteristic of theories with an internal length scale. Another consequence of the mesh-size cut-off is the introduction of an effective stacking fault energy. To see this, imagine a process of slip whereby two half crystals slide rigidly along a crystallographic plane. Under these conditions, the equipartition criterion causes the mesh to collapse towards the slip plane. The process of collapse ends when the mesh size h reaches the value $h_{\min}$. This results in an uniformly sheared cut plane of 'thickness' $h_{\min}$. The strain energy associated with the shearing deformation is periodic in the amount of slip. For simplicity, assume that the strain energy density passes through a single maximum $W_{\max}$ within each period. At the maximum, the crystal is in unstable equilibrium, and the energy per unit length of the cut plane is, evidently, $\gamma \sim W_{\max} h_{\min}$, which can therefore be interpreted as an effective stacking fault energy.

It is instructive to probe the limiting behavior of the theory at the atomistic microscale. Here the question is whether the theory can stably support lattice defects such as dislocations and, if so, how close are their cores to those predicted by an unconstrained atomistic simulation. A calculation of the core of a Lomer dislocation in aluminum is shown in Fig. 1. The atomistic potential adopted in the calculation is of the Embedded Atom type, as fitted to *ab initio* calculations by Ercolessi and Adams [3]. The initial displacements in the conjugate gradient iteration are set to the linear elastic solution. Fig. 1 compares the core obtained from the quasi-continuum method and a direct atomistic simulation.

Three aspects of the solution bear emphasis. Firstly, the ability of the theory to produce stable lattice defects is noteworthy. In particular, the theory enables the crystal to be cut along a crystallographic cut-plane and slipped by a translation vector of the lattice without any change in energy. Secondly, the dislocation is accorded a well-defined core energy, a manifestation of the existence of an intrinsic length scale in the theory. Thirdly, although not exact, the structure of the core is in reasonable agreement with the prediction of the atomistic simulation.

The example shown here is intended as a demonstration of the limiting behavior of the theory on the atomistic scale. Applications to problems in nanomechanics fit perhaps more naturally within the scope of the theory and will be pursued in a forthcoming publication [4]

The Nucleation of Dislocations at a Crystal Surface

The behavior of dislocations in materials intended for use in microelectronic devices has been a topic of long-standing interest because of the effect of dislocations on electronic properties of the materials. One example is the appearance of misfit dislocations in layers which have been epitaxially grown onto a substrate with a slightly different lattice parameter. Invariably, this process involves materials which have been chosen primarily for their electronic transport properties, and not for reasons related to lattice parameter or mechanical defect characteristics. The strain which arises through the constraint of epitaxy is commonly relieved by the formation of misfit dislocations at the interface between the strained layer and its substrate. If these dislocations are prevented from forming, the stress in the film is not necessarily detrimental; indeed, in some cases the influence of strain on band structure of the material can be exploited to some advantage in charge confinement in the system.

The appearance of misfit dislocations during epitaxial growth has been observed experimentally to coincide with the attainment of a critical thickness which, in turn, depends on the elastic

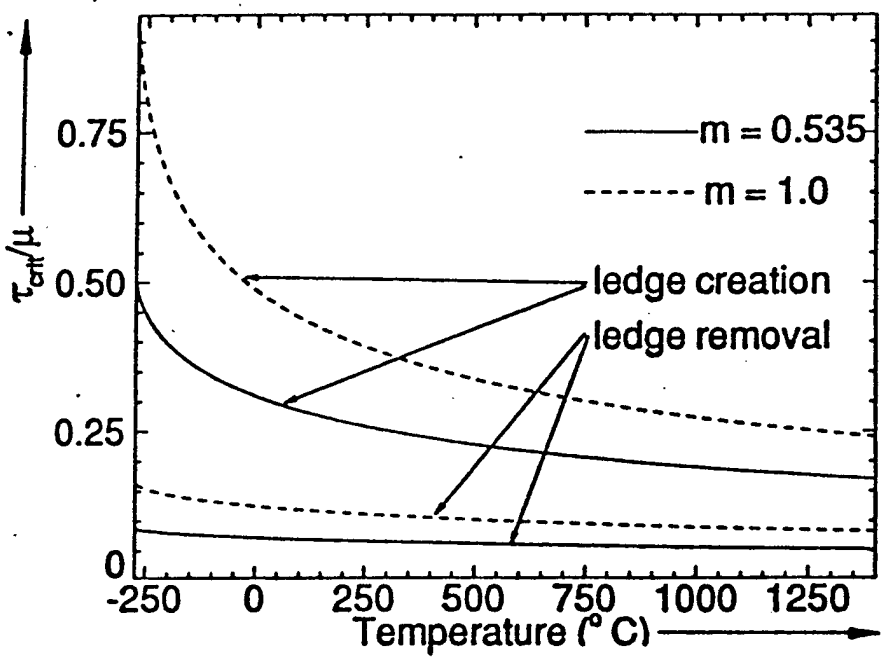

Fig. 2. The critical shear stress required to emit a dislocation for a free surface as a function of temperature.

mismatch strain, elastic constants, and crystallographic orientation. Theoretical studies of this problem have established the validity of the critical thickness concept, and the theory has been supported by very careful experiments. A persistent difficulty in this area is that, on the one hand, the critical thickness concept is based on the behavior of a pre-existing dislocation while, on the other hand, materials can be grown of such high crystalline quality that the population of pre-existing dislocations in insufficient to accommodate significant relaxation of the elastic mismatch strain. Thus, the nucleation of dislocations emerges as a problem of central importance in such systems.

Several mechanisms of dislocation nucleation in strained epitaxial films have been proposed. None seems to be present over a wide range of materials and/or conditions, and nucleation processes appear to be somewhat material specific. However, there is evidence to support the view that dislocations can be nucleated as loops at the growth surface of a strained material. It has been argued that the activation energy for this process is prohibitively large, and thus that the process is unlikely to occur. However, such models have been based on a restricted model of dislocation loop formation and on the role of the free surface.

We have reexamined the process of dislocation nucleation at a crystal surface in light of recent developments within the theory of nucleation [5]. An exact expression for the elastic energy associated with a semicircular shear dislocation loop emanating from a free surface has been obtained and compared with earlier approximations. It has been demonstrated that the energy of a half loop emanating from a free surface has the form

$$U^{\text{half}} = \frac{\mu b^2 r}{8} \frac{2-\nu}{1-\nu} \ln \frac{8mr}{e^2 r_0} \tag{6}$$

where μ is the shear modulus, ν is Poisson's ratio, b is the magnitude of the Burgers vector, r

is the radius of the half loop, r_0 is the core cut-off radius, e is the natural logarithm base, and m is a dimensionless parameter. It is noteworthy that, for $m = 1$, this expression gives one-half the energy of a *full* loop in an *unbounded* solid. The energy required to activate a semicircular dislocation loop into its unstable equilibrium configuration is then calculated on the basis of the modified self-energy estimate. As shown in Figure 2, the shear stress necessary to emit the loop, as a function of temperature, is almost 50% less than earlier estimates. Thus, when a more realistic description of a dislocation line is adopted, the process of surface nucleation of dislocation loops becomes much more plausible in such system.

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L. B. Freund

M. Ortiz

R. Phillips