Final Report
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LDA Calculations of Dislocation Mobility in Fe & Mo:

Final Report

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1 Abstract

This project was a collaborative effort between Murray Daw (Clemson) and Daryl Chrzan (LBNL/UCB). The main goal of this project was to accomplish the first-ever first-principles calculations of the structure of the screw dislocation in Fe and to study the effects of stress and magnetization. The calculations were completed and reported at conferences.

During the work on this project, the collaboration also tackled an important related question — the effect of periodic boundary conditions in dislocation calculations on the stress-state. The solution to the problem for this particular case has had much broader impact than the specific results of the calculation in iron. This technique was published in Computational Materials Science, and has been applied recently to the study of dislocations on nanotubes (submitted).

Finally, the collaboration considered the application of scaling formalism to a simple problem of dislocation emission from a single, stress-activated source. The result is a very elegant, compact solution to a simple textbook problem, which was published in Phil Mag. This result lays the foundation for continuing work on applying scaling formalism to dynamics of more complex dislocation problems.

2 Scientific progress

This project is a collaborative effort between Murray Daw (Clemson) and Daryl Chrzan (LBNL/UCB). The main goal of this project is to accomplish the first-ever first-principles calculations of the structure of the screw dislocation in Fe and to study the effects of stress and magnetization.

2.1 Screw dislocations in Fe

In the first year of this project, we obtained the optimized structure of the screw dislocation in Fe and Mo. Both the easy- and hard-core structures have been optimized (the hard-core was unstable for Mo). The calculations used the Generalized Gradient Approximation (GGA), and were based on the Projected Augmented Wave (PAW) scheme, both implemented in the Vienna Atomic Simulation Package (VASP). The energy and magnetization differences were obtained.

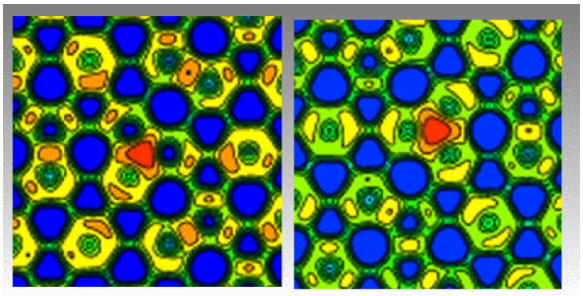

Figure 1: Calculated electron charge density for two forms of the screw dislocation core in Fe. At left is the "easy" core, at right the "hard".

We calculated the hard core in Fe to be 0.12 eV/Angstrom higher in energy than the easy core. In Mo the hard core was unstable. We also

calculated a change in the magnetic moment between the two core configurations. The hard core has a magnetic moment lower than the easy core by 1.8 Bohr-mag/Angstrom.

For the dislocation calculations, we used periodic boundary conditions, as usual for electronic structure calculations using a planewave basis. The dislocations were placed in a periodic quadrupolar array. The infinitely periodic array of dislocations places a stress on the individual cores, but a review of the literature turned up no prior work on a systematic method for calculating the stress in that case.

In order to establish the effects of the periodicity on the results, we have studied the problem of defects introduced into a periodic elastic medium. The results of that work has been submitted to Computational Materials Science for publications. This contribution has been used to analyze periodic dislocation arrays, and also dislocations on nanotubes.

2.2 Stress effects due to periodic boundary conditions in electronic structure calcualtions

We investigate the effects of elastic interactions between defects in electronic structure calculations with periodic boundary conditions. Our approach built on the work of Toshio Mura from 1964. In this formulation, the distortion tensor depends on the periodicity and the topology of the defects and does not involve evaluating sums of long-range functions. We construct solutions in a straight-forward way that makes them easily applied to electronic structure calculations. The results explain how to interpret volume changes in systems with periodic boundary conditions. We also show that the periodicity may be chosen in such a way as to minimize the elastic effects of the boundary condition.

The common use of periodic boundary conditions for electronic structure calculations naturally brings up questions about artifacts due to the boundaries. In particular, recent attention has been focused on the nature of the stress-fields produced by a periodic array of defects and how those may affect the calculations. This is an important issue, for example, in the examination of the effects of stress on dislocation mobility — which was the central topic of this project. One would like to know, and be able to control, the complete stress-state of a dislocation to examine how non-glide stress components may affect dislocation motion.

Recently several papers have appeared treating this problem by considering the strain field of a periodic array of defects to be a superposition of the strain fields for those defects isolated in an infinite medium. These superpositions must inevitably deal with issues of conditional convergence. However, the authors of those papers seem unaware of the work in the 60's by Toshio Mura. Mura's approach is very simple and leads immediately to complete solutions; furthermore, his approach also neatly avoids all issues of

conditional convergence.

Our approach is explained almost completely by stating that *at its equilibrium, the distortion minimizes the elastic energy subject to constraints imposed by the defect.* We impose periodic boundary conditions by noting that the distortion field is a periodic function of position and so can be expressed in a series of plane waves (a generalization of a Fourier Series). The elastic energy, which is quadratic in the distortion, is then represented in terms of an infinite sum over reciprocal lattice vectors. Thus, to form a complete solution, the distortion must match any topological conditions imposed by the defects, and any freedom left in the distortion must minimize the elastic energy in the cell.

This is enough to completely specify the solution. The solution is expressed as an infinite sum, but the sum can be shown to be absolutely convergent, in contrast to other recent solutions which involve carefully balancing opposing terms.

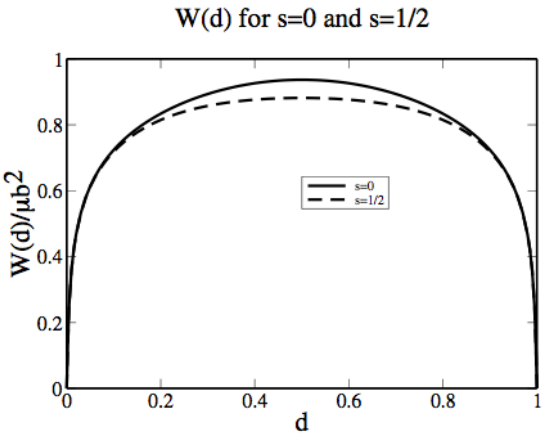

Figure 2: Elastic energy as a function of dipole separation in the periodic array. The curves are calculated for two different shaped cells, as described by a parameter s.

In Fig. 2, we show the elastic energy (per unit cell per length) as a function of dipole separation d for two values of cell offset s. Clearly for this geometry the dislocations are in unstable equilibrium for $d = 1/2$. If the dipole is allowed to collapse, the energy vanishes; this is possible because we have smeared the dislocation cores and so the annihilation of oppositely signed dislocations can occur without singularity. Likewise, expanding the dipoles beyond the equilibrium causes the members to annihilate with oppositely-signed partners from other periodic cells. One can show numerically that the energy depends logarithmically on r_s.

The resulting displacement fields are shown in Fig. 3.

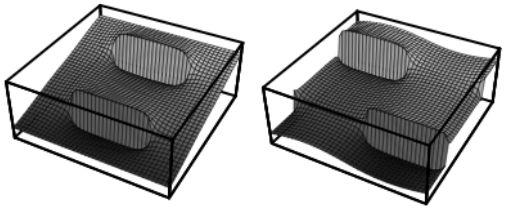

Figure 3: Displacement fields for a screw dipole, as illustrated for different periodic cells.

The periodic boundary condition imposes a stress on the dislocations which they would not have an infinite medium. This effect can be evaluated, and some of the result is shown in Fig. 4.

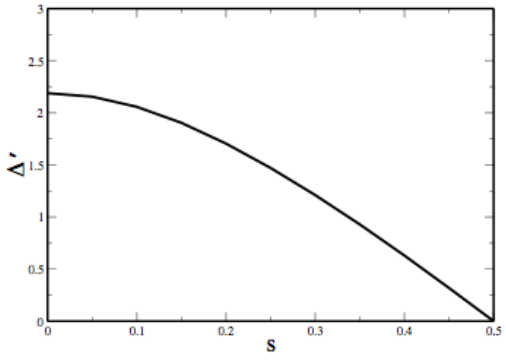

Figure 4: Gradient of a component of the stress on a dislocation due to periodicity, as a function of cell offset. For more details, see the publication.

This approach provides a systematic and unambiguous solution to the problem of periodic boundary conditions and defects. It provides initial positions for defect calculations, as well as an evaluation of the stress state of defects imposed by the periodic boundary conditions.

An unexpected benefit of the approach was to provide a foundation for treating dislocations on nanotubes, which can be viewed as cylindrically shaped elastic membranes. The cylindrical symmetry imposes a periodicity on the solutions in the cylindrical angle, and this is exactly what can be treated with our formulation. The advance was recognized immediately. Daryl Chrzan's student Elif Ertekin was able to work through the challenging theory of a curved elastic membrane. The resulting continuum theory of dislocations on nanotubes was compared directly to first-principles calculations of the same defects, and the results are impressive. The upshot is that continuum theory is more than adequate to provide an accurate description of

dislocation energetics on nanotubes. This has been submitted for publication in two forms (letter and longer paper).

In a parallel project, we have conducted a continuum study of the collective behavior of a dislocation array emitted from a single source. A novel scaling approach was applied, and the results of the analysis were compared to numerical simulations. Most of the theoretical work was accomplished by an advanced undergraduate working at Clemson. This work was published in Phil. Mag. Some progress was also made including finite-size effects.

2.3 Scaling in a simple model of dislocation activity

We examine a simple, 1-D model of dislocation activity, including a stress-activated source and mutually interacting dislocations. We demonstrate, through numerical and analytical steps, that the dislocations emitted from a 1-D stress-activated source evolve toward a distribution which is self-similar in time, and we derive the power-law forms and distribution function. We show that the asymptotic distribution is a step-function, and the dislocation front moves out linearly in time. The spacing between dislocations in the asymptotic distribution is uniform and increases logarithmically in time. The number of dislocations increases as $t/\ln(t)$, and the strain increases as $t^2/\ln(t)$.

A simple model of dislocation activity which addresses a stress-activated source of overdamped, interacting dislocations. An external stress σ is exerted on a source (at $x = 0$), which emits individual dislocations. The dislocations are emitted in pairs; the dislocations in $x > 0$ have burger's vector b, and in $x < 0$ have the opposite burger's vector $-b$. These equations of motion are coupled and therefore difficult to solve any way except numerically.

The discrete equations were integrated numerically with a straightforward approach, and the results demonstrated that the solution approach an intermediate asymptotic as anticipated. The scaling exponents were then obtained from the numerical results.

In the limit of a large number of dislocations, it should be possible to approach the same problem in terms of a continuum distribution function. The governing equation for that distribution was then solved, using the discrete numerical results as a guide, by applying scaling theory. The scaling law converts a non-linear partial differential equation into a non-linear ordinary eigenvalue problem, from which the scaling exponents were obtained analytically, in agreement with those obtained from the discrete simulations.

Recognizing the applicability of scaling behavior is a powerful tool for analyzing complex systems. We believe this behavior is characteristic of dislocation-source problems in general and expect that our approach should be useful in more complex systems.

3 Student involvement

One PhD student (Lingyun "Neil" Xu) learned various aspects of electronic structure calculations (using VASP), including density-of-states, band dispersion diagrams, and Nudged Elastic Band calculations. Clemson will award Mr. Xu his Ph.D. in Physics in August of 2007. (full support for one year)

Another grad student (Colin Harris) carried out the scaling analysis of the dislocation source in a finite medium. He was awarded his Master's degree in Physics from Clemson in 2006. (full support for one year)

An undergraduate student (Jack Deslippe) was also involved in much of the work. He received has Bachelor's degree in Physics from Clemson in 2005 and is currently a graduate student in Physics at UC Berkeley.

4 Publications (acknowledging support from this grant)

- M. S. Daw, "Elasticity Effects in Electronic Structure Calculations with Periodic Boundary Conditions", Computational Materials Science, v38 p293 (2006).

- J. Deslippe, R. Tedstrom, M. S. Daw, D. Chrzan, T. Neeraj, and M. Mills, "Dynamic scaling in a simple one-dimensional model of dislocation activity", Phil. Mag. 84, 2445-2454 (2004).

- E. Ertekin, M. S. Daw, and D. C. Chrzan, "Transferable description of the Stone-Wales defect formation energy in graphene and carbon nanotubes", (submitted 2007) (support for Daw)

- E. Ertekin, M. S. Daw, and D. C. Chrzan, "Topological description of the Stone-Wales defects in nanotubes", (submitted to Phys Rev 2007) (support for Daw)

5 Conference Presentations (acknowledging support from this grant)

- J. Deslippe [presenting], M. Daw, D. Chrzan, M. Mills, and N. Thirumalai, "DYNAMICAL SCALING IN A SIMPLE 1D MODEL OF DISLOCATION ACTIVITY" (contributed paper at 2004 Annual Meeting of the TMS).

- Murray S. Daw [presenting] and Daryl C. Chrzan, "FIRST-PRINCIPLES ELECTRONIC STRUCTURE OF SCREW DISLOCATIONS IN alpha-Fe" (contributed paper at 2004 Annual Meeting of the TMS).

- E. Ertekin [presenting], M. Daw, and D. Chrzan, "Continuum description of defects in carbon nanotubes" (contributed paper at 2007 March Meeting of the APS). (support for Daw)