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Atomic-Scale Modeling of the Structure and Dynamics of Dislocations in Complex Alloys at High Temperatures

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Abstract

We report on the progress made during the first year of the project. Most of the progress at this point has been on the theoretical and computational side. Here are the highlights:

- A new code, tailored for high-end desktop computing, now combines modern Accelerated Dynamics (AD) with the well-tested Embedded Atom Method (EAM).
- The new Accelerated Dynamics allows the study of relatively slow, thermally-activated processes, such as diffusion, which are much too slow for traditional Molecular Dynamics.
- We have benchmarked the new AD code on a rather simple and well-known process: vacancy diffusion in copper.
- We have begun application of the AD code to the diffusion of vacancies in ordered intermetallics.

1 Project Description

Developing a complete understanding of dislocation-level processes at high temperatures is crucial to the physically-based modeling of the creep performance of structural materials such as superalloys and intermetallics. However, there are presently several significant challenges which stand in the way of employing dislocation modeling concepts to the problem of high-temperature deformation in these complex alloys. First, the dislocation configurations at the atomic level can be far more complex at higher temperatures because of the additional degree of freedom offered by diffusion-mediated climb processes. Second, the diffusion paths are not accurately known, and are affected by the presence of the dislocation's core and strain field. Third, though alloying additions and deviation from stoichiometry can have dramatic effects on mechanical properties, their effects on fundamental dislocation configurations and microscopic diffusional processes are largely unknown.

In this program, we intend to develop a modeling capability at the atomic scale whereby we can rigorously treat the non-conservative motion of complex dislocation configurations, and obtain quantitative estimates of dislocation velocities - an essential first step toward the prediction of high temperature performance of structural materials. This effort is inspired by recent advances in these distinct areas:

- Improved understanding of dislocation processes controlling high-temperature deformation in complex intermetallics
- Revolutionary advances in the computation of the dynamics of thermally-activated processes

Specifically, the goals stated in our proposal were to develop a modeling capability which can:

- Compute atomic structures and mobilities of point defects and dislocations
- Flexibly employ and compare energy functions from a variety of models (particularly EAM and the more recently developed BFS method)
- Benchmark energetics of important processes from first principles
- Simulate atomic movement via diffusional processes near dislocations and obtain realistic rate information
- Treat the effects of alloying on the rates of diffusion and dislocation motion

The progress this year has concentrated on the modeling challenge. In particular, we have made significant advances in the computational tools used to study diffusion and have begun to use these tools in the study of vacancy diffusion in intermetallics.

2 This Year's Progress

We have combined modern accelerated dynamics with the Embedded Atom Method (EAM) to provide an advanced tool for investigating thermally activated processes (diffusion and dislocation climb) on an atomic scale. A new code, tailored for the current high-end desktop computing environment, now includes the accelerated dynamics.

When applied to diffusion, traditional Molecular Dynamics is constrained to follow the high-frequency vibrations of all the atoms in the system (with a typical period of picoseconds) which only rarely results in an atomic hop. By contrast, Accelerated Dynamics allows the study of relatively slow, thermally-activated processes, such as diffusion, in a much quicker and more revealing way. Our project has combined a robust algorithm which searches for saddlepoints (Dimer Method) with kinetic Monte Carlo, thereby integrating out the high-frequency motion and concentrating on the interesting atomic hops. Because the new method is so robust, it can be applied even to the dynamics of very complex processes.

In Kinetic Monte Carlo (kMC), the system begins in a local valley of the potential energy surface. For the system to move to a neighboring valley requires it to pass over one of possibly several saddlepoints. If the list of possible saddlepoints is known (and also the energy barrier Q for each), the kMC procedure picks one at random based on a Boltzmann weighting $\exp(-Q_i/kT)$. The system is then moved over that saddlepoint to the next valley, and the simulated time is calculated as proportional to $\exp(Q_i/kT)$.

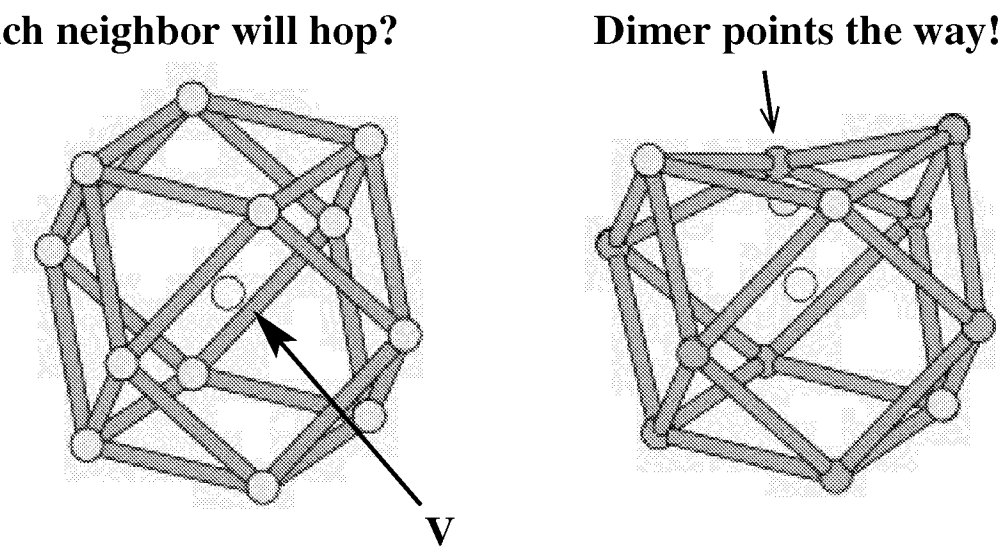
The Dimer Method is a scheme for finding saddlepoints on a high dimensional potential energy surface. To understand the scheme, consider that an arrangement of N atoms forms a point in $3N$-dimensional configuration space. From such a point in configuration space, one could calculate the curvature of the energy in all directions. A saddlepoint is a configuration which has exactly one direction with negative curvature, in contrast to a minimum where all directions have nonnegative curvature. When searching for a saddlepoint from a starting configuration, complete knowledge of the curvature in all directions would enable one to move toward the saddlepoint by focusing on the direction with the lowest (eventually negative) curvature.

The "Dimer" in the Dimer Method is formed by taking two neighboring points in configuration space (that is, two configurations which are slightly different). If the Dimer is allowed to rotate freely without translating in configuration space, the energy of the Dimer will be minimized when it points along the direction of lowest *curvature* in the energy. In the region near a saddlepoint, this is the direction of negative curvature, in contrast to all other directions which have positive curvature. In the simplest case, the dimer acts like a compass, pointing from a valley toward a saddlepoint. Even in more complex cases, the dimer direction can be used to move the dimer toward the saddlepoint. The numerical advantage of the dimer scheme is that some second derivative information is obtained, but only first derivatives are explicitly calculated from the potential surface.

The saddlepoint search in the Dimer Method must be started by selecting some initial orientation of the Dimer, and this should then lead to a saddlepoint. Once one saddlepoint is found, the Dimer Method must be started again with a different initial direction to locate another saddlepoint. Clearly, it is best to find some efficient means of providing profitable initial orientations for the dimer search. Also, to be efficient, the successive applications of

the Dimer Method should avoid rediscovering previously identified saddlepoints. With these thoughts in mind, we have made some improvements to the efficiency of the Dimer Method.

Consider as an example, the hop of a V in Cu, shown in the following figure. In *FCC* metals, there are 12 nearest neighbors to the vacancy. Applying the Dimer Method 12 times in succession comes up (in our code) with a new saddlepoint each time. This table of saddlepoints can then be used in the Kinetic Monte Carlo to decide which of the 12 neighbors will exchange places with the vacancy. In this fashion, we have combined *kMC* with the Dimer Method, and this has been implemented in *flame*.



Here is a summary of our key accomplishments for this year:

- new code (*flame*) for doing accelerated dynamics with EAM, tailored to Pentium architecture
- new functionalities are critical for current interests:
  - Dimer Method (robust saddlepoint search)
  - kinetic Monte Carlo (uses Dimer Method to find saddlepoints)
  - new Hyper-Dimer (original with this work)
- successful benchmark application to simple, well-known case (V in Cu)
- first runs for Ni vacancy in Ni_3Al

3 Code Description

The new code (*flame*) should replace commonly used but dated Sandia *dynamo* code, which was written (by Daw & Foiles in the late 80's and early 90's) for the Cray. *Dynamo* and its related codes have become commonly used throughout the community. The new code retains the easy usability that characterized the *dynamo* suite. In addition, *flame*'s execution of the

traditional functionalities (energy minimization, molecular dynamics, Langevin dynamics) is much faster than *dynamo*. There are several advances which give *flame* advantages in the current computing environment:

- The old code was targetted for smaller problems than are feasible today. The target systems are now larger.
- A significant improvement in the speed is attained by utilizing a "linklist" strategy for finding neighbors when calculating interactions. The code stores the neighbor lists from one iteration to the next, updating them only when necessary.
- Larger memories makes it possible to store several configurations simultaneously in memory. This is very convenient for constructing chains-of-state for saddlepoint searches, or tables of saddlepoints for *kMC*.

A working version of *flame* will be made available with this report to our contacts at NASA.

4 Plans for the coming year (2003)

4.1 Theoretical Portion

For the theoretical work, the target application of this project in the coming year will be:

1. the diffusion of vacancies in ordered intermetallics, and
2. the interaction of those vacancies with dislocations

Progress has been such that we anticipate reporting on the first round of results at the Intermetallic Symposium of the 2002 Fall Meeting of the MRS in Boston.

4.2 Complementary Experiments

Our success in the development of the accelerated molecular dynamics should enable us to begin treating diffusion and defect interactions with dislocations in systems of interest. We believe that a problem of significant interest from a fundamental and technological viewpoint is that of dislocation motion in the ordered γ' phase of Ni_3Al. Based on previous creep studies [T. S. Rong, I. P. Jones and R. E. Smallman, Acta Metall. Mater., vol. 43, (1995), pp. 1385-1393], deformation of single crystals of the γ' phase at intermediate temperature (500-700C) occurs by motion of $a\langle 110\rangle$ superdislocations. These dislocations are reported to adopt climb-dissociated configurations under these conditions, such that the $a/2\langle 110\rangle$ superpartials lie on top of one another relative to the overall glide plane. An APB links the two superpartials together in the ordered structure. It is the motion of such configurations that appears to limit deformation under these creep conditions.

We will perform detailed TEM investigation of such dislocation configurations to determine overall glide planes, dissociation distances and dislocation densities. Initial efforts

are planned to creep deform a limited number of $Ni_3(Al, Ta)$ crystals that are available, although additional compositions may be pursued in consultation with NASA personnel. This information will be used to obtain estimates of dislocation velocities that will enable us to benchmark the accelerated dynamics modeling of appropriate dislocation configurations using *flame*.

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