AFRL-RX-WP-TR-2013-0208

COLLABORATIVE RESEARCH AND DEVELOPMENT (CR&D) III
Task Order 0077: Fundamental Studies of Plasticity, Interfacial Boundaries and Liquid Metals

Dallas Trinkle
Independent Contractor

JUNE 2013
Final Report

AIR FORCE RESEARCH LABORATORY
MATERIALS AND MANUFACTURING DIRECTORATE
WRIGHT-PATTERSON AIR FORCE BASE, OH 45433-7750
AIR FORCE MATERIEL COMMAND
UNITED STATES AIR FORCE

NOTICE AND SIGNATURE PAGE

Using Government drawings, specifications, or other data included in this document for any purpose other than Government procurement does not in any way obligate the U.S. Government. The fact that the Government formulated or supplied the drawings, specifications, or other data does not license the holder or any other person or corporation; or convey any rights or permission to manufacture, use, or sell any patented invention that may relate to them.

This report was cleared for public release by the 88th ABW Public Affairs Office (Case Number: 88ABW-2013-4548, dated Oct 31, 2013) and is releasable to the National Technical Information Service (NTIS). It is available to the general public.

Qualified requestors may obtain copies of this report from the Defense Technical Information Center (DTIC) (http://www.dtic.mil).

AFRL-RX-WP-TR-2013-0208 HAS BEEN REVIEWED AND IS APPROVED FOR PUBLICATION IN ACCORDANCE WITH ASSIGNED DISTRIBUTION STATEMENT.

____//SIGNATURE//_____   __//SIGNATURE//_____
CHRISTOPHER WOODWARD, Project Engineer   DANIEL EVANS, Chief
Metals Branch   Metals Branch
Structural Materials Division   Structural Materials Division

_____//SIGNATURE//_____
ROBERT T. MARSHALL, Deputy Chief
Structural Materials Division
Materials and Manufacturing Directorate

This report is published in the interest of scientific and technical information exchange, and its publication does not constitute the Government's approval or disapproval of its ideas or findings.

REPORT DOCUMENTATION PAGE

1. REPORT DATE *(DD-MM-YY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
June 2013	Final	22 December 2009-31 May 2013

4. TITLE AND SUBTITLE
COLLABORATIVE RESEARCH AND DEVELOPMENT (CR&D) III
Task Order 0077: Fundamental Studies of Plasticity, Interfacial Boundaries and Liquid Metals

5a. CONTRACT NUMBER
FA8650-07-D-5800-0077

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
62102F

6. AUTHOR(S)
Dallas Trinkle

5d. PROJECT NUMBER
4347

5e. TASK NUMBER

5f. WORK UNIT NUMBER
X2100000

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Universal Technology Corporation
1270 N. Fairfield Road
Dayton, OH 45432-2600

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory
Materials and Manufacturing Directorate
Wright-Patterson Air Force Base, OH 45433-7750
Air Force Materiel Command
United States Air Force

10. SPONSORING/MONITORING AGENCY ACRONYM(S)
AFRL/RXCM

11. SPONSORING/MONITORING AGENCY REPORT NUMBER(S)
AFRL-RX-WP-TR-2013-0208

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES
PA Case Number: 88ABW-2013-4548; Clearance Date: 31 Oct 2013.

14. ABSTRACT (*Maximum 200 words*)
This research in support of the Air Force Research Laboratory Materials and Manufacturing Directorate was conducted from 22 December 2009 through 31 May 2013. The objective of this project was to explore fundamental structure-property relationships in structural metals using advanced first principles methods.

15. SUBJECT TERMS
thermally-activated slip, lattice green function calculation

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT:	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON (Monitor)
a. REPORT Unclassified	**b. ABSTRACT** Unclassified	**c. THIS PAGE** Unclassified	SAR	13	Christopher Woodward

19a. NAME OF RESPONSIBLE PERSON (Monitor)
Christopher Woodward

19b. TELEPHONE NUMBER *(Include Area Code)*
(937) 255-9816

TABLE OF CONTENTS

1.0   SUMMARY

During the contract period, we began work on the adaptation of a thermally-activated kink-pair model from HCP metals to BCC metals. This model was based on previous work on HCP metals [Yasi2011], that was in itself adapted from an earlier model [Trinkle2005]. While the previous 2005 model was designed for BCC metals, the 2011 computational model removed many of the assumptions and simplifications of the 2005 model, and so the goal was to begin work on repurposing the later model to the specific geometry of an screw dislocation in BCC metals, such as Mo and Fe, to be used for the study of solid-solution strengthening and softening in low temperature deformation.

In addition to beginning the work on slip modeling, part-way through the contract period, we began work on the calculation of the lattice Green function for Ni and Ni_3Al using data provided by Dr. Chris Woodward at AFRL, to be evaluated using the algorithms laid out in [Trinkle2008] and [Yasi2012]. The resulting lattice Green functions can be used in a modified version of VASP for flexible-boundary condition calculations.

2.0   INTRODUCTION

2.1   Thermally-Activated Slip in HCP and BCC Metals

In some body-centered cubic metals, solutes decrease the strength of the material. This effect, known as solid-solution softening, is a reduction in the stress at which a material begins to deform irreversibly (yield stress) or as a reduction in the material's ability to resist indentation (hardness). Softening is important for producing viable materials: The bcc refractory metals (Nb, W, Ta, and Mo) offer a possible new class of high-temperature materials for turbine-engine or nuclear power plant components, but have poor low-temperature behavior in elemental form. As the temperature decreases from 15% of the melting temperature (above room temperature for Mo, W, etc.) down to absolute zero, strength increases rapidly. This high strength is undesirable, because it is linked with an increase in fracture and low malleability, ultimately limiting the use of these materials as critical structural components. Classical metallurgical practice is to reduce this risk by incorporating solid-solutions, or by introducing new softer phases. Models have only succeeded in qualitatively explaining the possibility of low temperature softening, or in finding empirical correlations to deduce scaling trends. More recent work was able to quantitatively predict the change in flow stress in Mo alloys with solute type, concentration, and temperature [Trinkle2005].

This work was recently extended to another crystallographic system with thermally-activated deformation: cross-slip from basal to prismatic in magnesium alloys with the addition of solutes. The computational model to describe this behavior relies on (a) an accurate description of the dislocations involved in deformation, (b) their change from one core structure to another via kinks, (c) the interaction between dislocations and solutes from first-principles data, and (d) the distribution of solutes to produce statistical averages of kink enthalpies. An earlier model for BCC metals [Trinkle2005] used a series of approximations to (b) and (d) to produce a computationally tractable model. The more recent model of [Yasi2011] removed these approximations in favor of direct calculation of dislocation kinks and distribution of solute energetics. This forms the basis for updating the BCC solid-solution model.

2.2   Lattice Green Function Calculation of Ni and Ni_3Al

Flexible boundary conditions use the perfect lattice Green function to relax the forces on atoms near a defect by coupling to an infinite bulk; in this way, simulation of a defect requires only a small number of atoms near the defect geometry, while the lattice Green function determines the displacement of bulk-like atoms away from the defect. The lattice Green function gives displacements in response to the Kanzaki forces near the defect in the harmonic limit. This gives an accurate treatment of the long-range stress field of a defect (such as a dislocation) while using *ab initio* forces close to the defect. Since the perfect lattice Green function has translational symmetry, it provides the "flexibility" in flexible boundary conditions: bulk lattice response is simulated *without* specifying an origin for the lattice. Moreover, using *ab initio* for the forces and the lattice Green function ensures accurate coupling of the defect region to infinite bulk without the mismatch of coupling classical potentials with *ab initio*.

Flexible boundary conditions are limited by the accuracy of the lattice Green function. Many closed-form results are known for the lattice Green functions of cubic lattices with nearest neighbor interactions. While the lattice Green function is intimately related to the elastic constants and force constant matrix of a crystal, it has previously been computed for realistic

potentials from relaxation of atom positions given an applied force. Rao *et al.* employed a "direct displacement" technique where separate relaxation calculations in a two-dimensional slab are used to numerically evaluate the lattice Green function for short range, while switching to the known long-range behavior of the elastic Green function. Woodward *et al.* used this same technique with *ab initio* for Mo, Ta, and TiAl, and found the lattice Green function matched the long-range behavior at distances of only 5Å, despite long-range metallic bonding. However, this technique is dependent on the defect geometry—a lattice Green function computed for a [110]/2 FCC screw dislocation cannot be used for the FCC edge dislocation with a threading direction of [112]/2. Moreover, relying on atomic relaxation can be prone to error in density-functional methods when the applied forces become small. Recently, we developed an accurate and computationally efficient approach instead relies on the force constant matrix and elastic constants, which can be computed using standard techniques, for single atom lattices [Trinkle2008] and multiple atom crystals [Yasi2012].

3.0   METHODS, ASSUMPTIONS, AND PROCEDURES

3.1   Thermally-Activated Slip in HCP and BCC Metals

We began work on the adaptation of a thermally-activated kink-pair model from HCP metals to BCC metals. A previously developed model for thermally-activated cross-slip in HCP Mg [Yasi2011] describes the thermally-activated cross-slip of a basal screw dislocation onto the prismatic slip plane. In HCP Mg, prismatic slip requires the nucleation of a pair of kinks (constrictions of a basal screw dislocation which glides one lattice plane in the prismatic plane) and migration down the length of a dislocation. This process is modified by the presence of solutes which both cause a distribution of different kink formation energies and barriers for kink motion along the length of the line. In BCC metals, such as Mo and Fe, screw dislocations move via a similar thermally-activated process of kink nucleation and migration; a simplified model of this process was used in an earlier publication [Trinkle2005]. The newer model for HCP makes use of direct calculation of solute distribution to predict the distribution of kink nucleation and migration barriers directly, as well as to include the effects of more complex solute distributions.

Current work involves the modification of the previous model for the specific dislocation geometry of a Mo screw dislocation core. This includes accounting for the screw dislocation kink geometry from classical potential simulations (needed to determine the size of the solute distribution region to be considered for the nucleation of kink-pairs). The previous simulation code is being modified to include the ⟨111⟩ screw dislocation core geometry with the distribution of site energy differences. This code will then be able to directly compute distribution of double kink nucleation energies as a function of solute concentration and type (where solute type is defined by the interaction energies of solute with a dislocation core); this will then be used to determine the BCC Mo-X Peierls stress as a function of temperature and solute concentration for a given plastic strain rate.

3.2   Lattice Green Function Calculation of Ni and Ni$_3$Al

The calculation of the lattice Green function for Ni and Ni$_3$Al uses the algorithms laid out in [Trinkle2008] and [Yasi2012]. The density-functional theory data are provided by Dr. Chris Woodward at AFRL. The lattice Green function data, in the form of input for a modified version of VASP, will be provided to AFRL. This provides necessary input for electronic structure calculation of Ni and Ni$_3$Al dislocation cores using flexible boundary conditions.

Approved for public release; distribution unlimited.

4.0   RESULTS AND DISCUSSIONS

4.1   Thermally-activated Slip in HCP and BCC Metals

Each nucleated pair of kinks in a solute field requires a total energy equal to the formation energies plus the change due to the presence of solutes in the kink; the distribution can be computed numerically. Each kink has a fixed number of sites in the core of the kink that may be occupied by solute atoms; we assume that the total energy change for the kink is the sum of all the individual energy changes, which are given by the site occupancy (either 0 or 1) multiplied by the energy of that site. We assume translational invariance down the length of the kink, so that there is unique set of site energies to consider, and along the row of a kink a set number of sites may be occupied with solute. Computationally, we can compute the distribution of solute/dislocation interaction energies, and produce a "density of states"-like expression for the probability of a given kink energy being encountered.

Solutes "roughen" the energy landscape for kinks and provide two barriers to the motion of kinks: a minimum (athermal) stress required for kinks to migrate preferentially down the dislocation line, and the energy barrier over the length of a kink. Solutes provide local changes in energy as a kink moves over a single Burgers vector; a minimum stress is necessary to overcome this short-range change in energy. This is given by the average roughness of the energy landscape: the energy changes as sites with solutes "leave" the kink and other sites "enter" the kink; the energy change for solutes entering is added, and subtracted for those leaving. The width of the solute interaction can be approximated as a Gaussian with area given by the Burgers vector squared and the stress to overcome is proportional to the energy difference. Analytically, we consider a distribution of energy differences as the sum of random variables for the energies; however, both addition and subtraction are equally likely so the mean is 0—that is, there are just as many "uphill" as "downhill" barriers. Together, we can compute "density of states"-like expressions for the probability of a given kink energy barrier being encountered, as well as an athermal stress to be overcome.

4.2   Lattice Green Function Calculation of Ni and Ni$_3$Al

The procedure for numerical computation of the lattice Green function in real space separates the Fourier transform into pieces which can be inverse Fourier transformed accurately. The straightforward approach would be to discrete inverse Fourier transform the inverse of the dynamical matrix; however, this transform converges very slowly with increased grid spacing due to the second-order pole at the gamma point. The inversion of the dynamical matrix to compute the lattice Green function is still best performed in reciprocal space, where the large R behavior is exactly contained in the pole at $k=0$. To accurately compute the lattice Green function requires an analytic treatment of the small k behavior separated from the rest of the Brillouin zone. The separation of the lattice Green function allows a discrete inverse Fourier transform to converge by analytically treating the second-order pole and discontinuity at $k=0$.

5.0   CONCLUSIONS

5.1   Thermally-activated Slip in HCP and BCC Metals

For magnesium, we have been successful at computing the change in cross-slip stress as a function of temperature, solute chemistry and composition. The modification to the algorithm—solute distributions, kink energetics—for BCC metals continues apace. The primary hurdles remain determining the kink geometry, and the incorporation of solute-solute interaction energies. In the case of HCP cross-slip in magnesium, the primary ingredient is the change in dislocation core geometry which could be treated as a discrete event (either basal or prismatic core configurations) while in BCC thermally-activated slip, the kink is transitioning from one screw dislocation core site to another, through a continuous change in slip. This leads to complications in determining the correct site energy to use in changing from the double kink formation energy in a BCC screw dislocation core. More work is required to produce a reliable model for BCC thermally-activated slip to replace the [Trinkle2005] model.

5.2   Lattice Green Function Calculation of Ni and Ni$_3$Al

The calculation of lattice Green functions for dislocations in Ni and Ni$_3$Al is concluding as expected, with the production of input for VASP flexible boundary condition calculations.

Approved for public release; distribution unlimited.

6.0   RECOMMENDATIONS

6.1   Thermally-activated Slip in HCP and BCC Metals

The development of a model that incorporates the new developments of the [Yasi2011] model for thermally-activated slip in BCC metals, a la [Trinkle2005], will require more work and testing to determine the best approach to dealing with intermediate configurations in the dislocation kink.

6.2   Lattice Green Function Calculation of Ni and Ni$_3$Al

The lattice Green function calculations performed as expected.

7.0 REFERENCES

[1]   [Yasi2011] J.A. Yasi, L.G. Hector, Jr., and D.R. Trinkle. Acta mater. **59**, 5652–5660 (2011), doi://10.1016/j.actamat. 2011.05.040.

[2]   [Trinkle2005] D.R. Trinkle and C. Woodward, Science **310**, 1665–1667 (2005), doi://10.1126/science.1118616.

[3]   [Trinkle2008] D.R. Trinkle, Phys. Rev. B **78**, 014110 (2008), doi:10.1103/PhysRevB.78.014110.

[4]   [Yasi2012] J.A. Yasi and D.R. Trinkle. Phys. Rev. E **85**, 066706 (2012), doi:10.1103/PhysRevE.85.066706.

LIST OF SYMBOLS, ABBREVIATIONS, AND ACRONYMS

Acronym	Description
AFRL	Air Force Research Laboratory
BCC	body center cubic
CR&D III	Collaborative Research and Development III
DOD	Department of Defense
DTIC	Defense Technical Information Center
FCC	face centered cubic
HCP	hexagonal close packed
EAR	Export Administration Regulation
ITAR	International Traffic in Arms Regulation
RX	Materials and Manufacturing Directorate
RXC	Structural Materials Division
RXCM	Metals Branch
USAF	United States Air Force
WPAFB	Wright-Patterson Air Force Base