STUDY OF THE EMBEDDED ATOM METHOD OF ATOMISTIC
CALCULATIONS FOR METALS AND ALLOYS

An Annual Progress Report
Current Budget Period:
March 1, 1990 - February 28, 1991

Submitted to:

Ms. Susan G. Hiser
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Submitted by:

R. A. Johnson
Professor of Materials Science

Report No. UVA/527359/MS91/102
October 1990

PREPARED FOR THE U. S. DEPARTMENT OF ENERGY
UNDER GRANT NO. DE-FG05-86ER45246

DEPARTMENT OF MATERIALS SCIENCE

SCHOOL OF
ENGINEERING
& APPLIED SCIENCE

University of Virginia
Thornton Hall
Charlottesville, VA 22903

OCT 31 1990

MASTER

UNIVERSITY OF VIRGINIA
School of Engineering and Applied Science

The University of Virginia's School of Engineering and Applied Science has an undergraduate enrollment of approximately 1,500 students with a graduate enrollment of approximately 600. There are 160 faculty members, a majority of whom conduct research in addition to teaching.

Research is a vital part of the educational program and interests parallel academic specialties. These range from the classical engineering disciplines of Chemical, Civil, Electrical, and Mechanical and Aerospace to newer, more specialized fields of Applied Mechanics, Biomedical Engineering, Systems Engineering, Materials Science, Nuclear Engineering and Engineering Physics, Applied Mathematics and Computer Science. Within these disciplines there are well equipped laboratories for conducting highly specialized research. All departments offer the doctorate; Biomedical and Materials Science grant only graduate degrees. In addition, courses in the humanities are offered within the School.

The University of Virginia (which includes approximately 2,000 faculty and a total of full-time student enrollment of about 17,000), also offers professional degrees under the schools of Architecture, Law, Medicine, Nursing, Commerce, Business Administration, and Education. In addition, the College of Arts and Sciences houses departments of Mathematics, Physics, Chemistry and others relevant to the engineering research program. The School of Engineering and Applied Science is an integral part of this University community which provides opportunities for interdisciplinary work in pursuit of the basic goals of education, research, and public service.

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DE91 001640

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ABSTRACT

Two projects were completed in the past year. The stability of a series of binary alloys was calculated using the embedded-atom method (EAM) with an analytic form for two-body potentials derived previously. Both disordered alloys and intermetallic compounds with the $L1_0$ and $L1_2$ structures were studied. The calculated heats of solution of alloys of Cu, Ag, Au, Ni, and Pt were satisfactory, while results for alloys containing Pd were too high. Atomistic calculations using the EAM were also carried out for point defects in hcp metals. By comparison with results in the literature, it was found that many body effects from the EAM significantly alter predicted physical properties of hcp metals. For example, the EAM calculations yield anisotropic vacancy diffusion with greater vacancy mobility in the basal plane, and imply that diffusion will start at a lower fraction of the melting temperature.

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TECHNICAL PROGRESS IN THE PAST YEAR

The heats of solution of disordered phases and $L1_2$, A_3B and $L1_0$ AB stoichiometric compounds have been determined for 12 binary alloys of fcc metals with atomistic calculations using an embedded-atom method (EAM) model. The analytic EAM model contains no adjustable parameters and is based on alloy potentials developed during the previous year. The heats of formation are in good agreement with ab initio calculations for Cu-Ag and Cu-Au but are somewhat high for Ag-Au. The heats of formation of Cu, Ag, and Au with Ni also show good agreement, with Pt are slightly high, and with Pd are significantly high. The $L1_0$ structure is tetragonal and the calculated c/a ratio of 0.89 for Cu-Au is close to the experimental value of 0.93. The rationale for developing the EAM is to be able to investigate problems that involve large numbers of atoms under complex conditions, i.e., cases that cannot be approached by ab initio calculations. The agreement with calculations which require many orders of magnitude more computing time indicates the present simple EAM model contains much of the essential physics required to represent alloying atomistically. This work has been published in The Physical Review.

Many-body effects on calculated defect properties in hcp metals were studied with an EAM model. The model parameters were determined by fitting to the atomic volume, cohesive energy, vacancy formation energy, and approximate elastic constants of titanium, while constraining the c/a ratio to the ideal value. The results were significantly different from published calculations with a model fitted to the same physical quantities but based on two-body forces and global volume dependence. Here vacancy diffusion was anisotropic rather than isotropic with greater mobility in the basal plane, and the vacancy migration energy was about half the vacancy formation energy rather than just 14 percent less. The divacancy migration energy was only about 10 percent less than that for single vacancies and divacancy binding was approximately isotropic. The stable interstitial consisted of an extra atom in the basal plane midway between two octahedral sites. The interstitial migration process was complex and anisotropic with activation energies less than those for vacancy migration. The primary conclusion is that local many-body effects are important in atomistic point defect calculations in hcp metals. This work was presented at a conference at the International Center for Theoretical Physics, Trieste, Italy, and has been accepted for publication in The Philosophical Magazine.

PUBLICATIONS FROM THIS GRANT (4.5 YEARS)

1. R. A. Johnson, "Interatomic Potential Development in Materials Science", in Computer Simulation in Materials Science, eds. R. J. Arsenault, J. R. Beeler, Jr., and D. M. Esterling (ASM, Metals Park, OH, 1987), p. 29.
2. R. A. Johnson, "Analytic Nearest-Neighbor Model for FCC Metals", *Physical Review B* **37**, 3924 (1988).
3. R. A. Johnson, "Relationship between Defect Energies and Embedded-Atom-Method Parameters", *Physical Review B* **37**, 6121 (1988).
4. D. J. Oh and R. A. Johnson, "Simple Embedded Atom Method Model for FCC and HCP Metals", *J. Materials Research* **3**, 471 (1988).
5. D. J. Oh and R. A. Johnson, "Embedded Atom Method Model for Close-Packed Metals", in Atomistic Simulation of Materials, eds. V. Vitek and D. J. Srolovitz (Plenum, New York, NY, 1989), p. 233.
6. D. J. Oh and R. A. Johnson, "A Semi-Empirical Potential for Graphite", in Atomic Scale Calculations in Materials Science, eds. J. Tersoff, D. Vanderbilt, and V. Vitek (Symposium Proceedings Volume 141, Materials Research Society, Pittsburgh, PA, 1989), p. 51.
7. R. A. Johnson and D. J. Oh, "Analytic Embedded Atom Method Model for BCC Metals", *J. Materials Research* **4**, 1195 (1989).
8. R. A. Johnson, "Alloy Models with the Embedded-Atom Method", *Physical Review B* **39**, 12554 (1989).
9. D. J. Oh and R. A. Johnson, "Relationship between c/a Ratio and Point Defect Properties in HCP Metals", *J. Nuclear Materials* **169**, 5 (1989).
10. R. A. Johnson, "Implications of the Embedded-Atom Method Format", in Many-Atom Interactions in Solids, (Springer-Verlag, New York, 1990), p. 85.
11. R. A. Johnson, "Phase Stability of FCC Alloys with the Embedded-Atom Method", *Physical Review B* **41**, 9717 (1990).
12. R. A. Johnson, "Many Body Effects on Calculated Defect Properties in HCP Metals", *Philosophical Magazine* (to be published).

STUDENTS

Two students are presently supported under this grant.

Jeanne R. Brown started work under this grant in July, 1989, as a Masters of Science candidate. Estimated date for completion of requirements leading to a Masters of Science degree is May, 1991. Jeanne worked seven years as a welder before returning to school, first to Monroe Community College in Rochester, NY, and then to Cornell University, where she received a Bachelor of Science degree in Materials Science and Engineering in May, 1988.

Zhan Yang started work under this grant in August, 1990, as a Masters of Science candidate. Estimated date for completion of requirements leading to a Masters of Science degree is May, 1992. Zhan graduated from Peking University, Beijing, China, with a BS in Physics in July, 1989 and spent a year at Alabama A & M prior to coming to Virginia.

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