SANDIA REPORT

SAND99-8207

Unlimited Release

Printed December 1998

Numerical Modeling of the Stability of Face-Centered Cubic Metals with High Vacancy Concentration

RECEIVED
APR 29 1999
OSTI

Brian P. Somerday, M. I. Baskes

Prepared by

Sandia National Laboratories

Albuquerque, New Mexico 87185 and Livermore, California 94550

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

Approved for public release; further dissemination unlimited.

Sandia National Laboratories

Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.

NOTICE: This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof, or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof, or any of their contractors.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Prices available from (615) 576-8401, FTS 626-8401

Available to the public from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Rd
Springfield, VA 22161

NTIS price codes
Printed copy: A03
Microfiche copy: A01

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

NUMERICAL MODELING OF THE STABILITY OF FACE-CENTERED CUBIC METALS WITH HIGH VACANCY CONCENTRATIONS

Brian Somerday and M. I. Baskes
Materials Reliability Department
Sandia National Laboratories/California

ABSTRACT

The objective of this research is to assess the possibility of forming an atomically porous structure in a low-density metal, e.g., Al with vacancies up to 0.20/lattice site; and to examine the effects of hydrogen and vacancy concentration on the stability of an atomically porous structure that has been experimentally produced in nickel. The approach involves numerical modeling using the Embedded-Atom Method (EAM). High vacancy concentrations cause the Al lattice to disorder at 300K. In contrast, Ni retains the face-centered-cubic structure at 300K for vacancy concentrations up to 0.15 Vac/lattice site. Unexpectedly, the lattice with 0.15 Vac/lattice site is more stable than the lattice with 0.10 or 0.20 Vac/lattice site. The Ni systems with 0.10 and 0.15 Vac/lattice site exhibit domains consisting of uniform lattice rotations. The Ni lattice with 0.15 Vac/lattice site is more stable with an initial distribution of random vacancies compared to ordered vacancies. The equilibrium lattice structures of Ni and Al containing vacancies and H are less ordered compared to structures with vacancies only at 300K.

This page intentionally left blank

NUMERICAL MODELING OF THE STABILITY OF FACE-CENTERED CUBIC METALS WITH HIGH VACANCY CONCENTRATIONS

Introduction

Experimental studies have shown that vacancy concentrations (0.15 to 0.25/lattice site) several orders of magnitude higher than thermal equilibrium values were produced in Ni, Ti, Pd, and Pd-Rh by conjoint application of high-pressure hydrogen gas (5 GPa) and elevated temperature ($>0.4T_m$) [1-5]. Vacancy generation is favored in face-centered-cubic (FCC) metal hydrides because of large hydrogen-vacancy binding energies coupled with numerous binding sites (6 per vacancy) [3]. “Superabundant” vacancies were distributed as point defects in the metal hydride and appeared to order on one simple-cubic sub-lattice to form an $L1_2$ -type structure [1-3]. The ordered defect structure was retained following intermediate-temperature annealing to off-gas hydrogen and subsequent cooling to room temperature [1]. Although this experimental evidence suggesting formation of stable defect structures is convincing, unresolved issues remain. For example, it is uncertain whether ordered defect structures would be stable in the complete absence of lattice hydrogen.

The atomically porous structure formed by superabundant vacancy generation in metal hydrides may be exploited to develop hydrogen storage materials. Hydrogen-fueled power supplies require light-weight hydrogen storage systems that can operate near ambient temperature. Atomically porous materials may offer both weight savings as well as accelerated hydrogen kinetics at low temperature compared to materials currently being considered for hydrogen storage applications. The possibility of forming stable defect hydride structures in low-density metals has not been explored, and hydrogen diffusion in atomically porous materials has not been characterized at ambient temperatures.

The objective of this research is to assess the possibility of forming atomically porous structures in a low-density metal, e.g., Al, and to examine the effects of hydrogen and vacancy concentrations on defect structure stability in a system that has been experimentally characterized, e.g., Ni. In addition, the kinetics of hydrogen diffusion at ambient temperature are investigated in atomically porous lattices. The approach involves numerical modeling using the Embedded-Atom Method (EAM) [6, 7]. Minimization of total energy as well as molecular dynamics and Monte Carlo simulations are used to assess lattice stability and hydrogen mobility in Al and Ni containing high vacancy concentrations.

Computational Procedures

Modeling simulations were performed on FCC lattices of Al and Ni that consisted of 1000 unit cells (4000 atom sites). Four vacancy (Vac) concentrations were considered for both Al and Ni: 0.05 Vac/lattice site (3800 atoms), 0.10 Vac/lattice site (3600 atoms), 0.15 Vac/lattice site (3400 atoms), and 0.20 Vac/lattice site (3200 atoms). Vacancies were initially distributed as point defects in two distinct arrangements at each concentration; i.e., vacancies were either randomly located on FCC lattice sites or ordered on one simple-cubic sub-lattice. Computations were performed on the Al-Vac and Ni-Vac systems as well as on defect structures containing lattice hydrogen (H). Hydrogen was placed in octahedral interstitial sites at concentrations from 0.50 to 1.0 H/solvent atom in Al and Ni lattices containing vacancy concentrations from 0.10 to 0.20 Vac/lattice site. The combination of H and vacancy concentrations considered were consistent with models that predicted vacancy concentration as a function of H content for different vacancy formation and binding energies [8].

All simulations were performed on lattices with periodic boundary conditions. Energy minimizations calculated the total potential energy of each lattice in the absence of kinetic energy; *viz*, temperature equaled 0K. The inputs for molecular dynamics (MD) simulations were lattices derived from energy minimizations. Molecular dynamics calculations were conducted at 300K over a simulated time period from 0.5 to 1.0 picoseconds. The inputs for Monte Carlo (MC) simulations were final results from the MD computations. Monte Carlo calculations were performed under fixed volume at 300K until the total energy of the system reached a constant value (after 10^6 to 10^7 steps).

The EAM potentials used in this study were developed for the Ni/Al/H system described in Refs. [9-11]. The functions were derived from the solubility and diffusivity of H in Ni and Al and the surface properties of H on Ni and Al. The elastic constants predicted from the EAM functions agree with experimental results for Ni and Al.

The stability of the FCC structures of Ni and Al was assessed through radial distribution functions of the lattices subjected to energy minimizations, MD simulations, and MC simulations. The radial distribution function (RDF) calculations show the number of neighbors at a distance (r) surrounding each atom in the lattice. Peaks in the RDF correspond to first-nearest neighbors, second-nearest neighbors, etc. as distance, r , increases.

Results and Discussion

Effects of Vacancy Concentration and Temperature

Increasing the vacancy concentration in Al from 0 Vac/lattice site to 0.20 Vac/lattice site systematically degrades the FCC crystal structure. Figure 1 shows the RDFs calculated for Al after energy minimization (corresponding to 0K) of the lattice. The RDF for 0 Vac/lattice site yields the expected result of delta functions at positions corresponding to first-nearest neighbors through fifth-nearest neighbors. The RDFs for Al containing 0.10, 0.15, and 0.20 Vac/lattice site consist of broad peaks distributed around the nearest-neighbor positions of the vacancy-free lattice. As the vacancy concentration increases from 0.10 to 0.20 Vac/lattice site, the RDF peaks become broader. In addition, the position of the maximum in the first-nearest neighbor peak is shifted to smaller distances due to the inward relaxation of atoms around a vacancy. These features indicate that increasing vacancy concentration degrades the crystallinity of Al. Distinct peaks are discerned at each nearest-neighbor position for 0.10 and 0.15 Vac/lattice site, suggesting that the FCC structure is retained at these vacancy concentrations. The FCC structure is lost for 0.20 Vac/lattice site.

Temperature causes a loss of crystallinity in Al for all vacancy concentrations. Figure 2 shows the RDFs calculated for Al based on MD simulations at 300K. The RDF for 0 Vac/lattice site shows peak broadening due to atomic vibrations. The RDFs for Al containing 0.15 and 0.20 Vac/lattice site exhibit discernible peaks only at the position for first-nearest neighbors, indicating that the FCC structure has been completely degraded. The RDF for 0.10 Vac/lattice site suggests that some FCC structure has been retained for this vacancy concentration, as mild peaks are observed at the third- and fifth-nearest neighbor positions.

Examination of RDFs for the Ni-Vac system shows both similar and contrasting features compared to the Al-Vac system at 0K. Figure 3 shows that the vacancy-free case consists of delta functions at the first-nearest neighbor through fifth-nearest neighbor positions, while addition of vacancies up to 0.20 Vac/lattice site causes peak broadening. In addition, the FCC structure is well defined for 0.10 and 0.15 Vac/lattice site but not for 0.20 Vac/lattice site. In contrast to the results for Al-Vac in Fig. 1, the FCC structure for Ni-Vac is not systematically degraded as vacancy concentration increases. Rather, lattice stability is enhanced at 0.15 Vac/lattice site. This is demonstrated in Fig. 3 by the higher peak heights for the RDF corresponding to 0.15 Vac/lattice site compared to 0.10 Vac/lattice site. (The lattice containing 0.15 Vac/lattice site consists of 3400 atoms, while the lattice containing 0.10 Vac/lattice site consists of 3600 atoms.)

The idea that lattice stability is enhanced for Ni-0.15 Vac/lattice site is supported by calculations of total potential energy at 0K. Figure 4 shows that a plot of energy per Ni atom vs the number of vacancies per lattice site exhibits a local minimum for the case of 0.15 Vac/lattice site.

The lattice structures for the cases of 0.10 and 0.15 Vac/lattice site exhibit unique features compared to the system with 0.20 Vac/lattice site. Figure 5(a) shows the atom positions

after energy minimization at 0K in Ni-0.15 Vac/lattice site for the orientation indicated. This figure shows that many rows of atoms are not parallel to the $\langle 100 \rangle$ axes. Rather, the lattice is characterized by a domain structure, where each domain consists of a uniform lattice rotation. The rows of atoms in the domains marked by arrows in Fig. 5(a) are brought into coincidence with the [001] axis by a 3° rotation around the [010] axis (Fig. 5(b)). Such lattice rotations were not pronounced for Ni containing 0.20 Vac/lattice site. The domain structure is also reflected in the RDFs for Ni-0.10 Vac/lattice site and Ni-0.15 Vac/lattice site in Fig. 3. The third-nearest neighbor through fifth-nearest neighbor peaks in these RDFs show distinct shifts to lower distances compared to the vacancy-free lattice, while the first- and second-nearest neighbor peaks are coincident with the vacancy-free lattice peaks.

The Ni-Vac system exhibits superior lattice stability compared to the Al-Vac system at a temperature of 300K. Figure 6 shows the RDFs calculated for Ni based on MD simulations at 300K. Unlike the RDFs for Al in Fig. 2, the results for Ni in Fig. 6 show that distinct peaks are discernible at each nearest neighbor position for vacancy concentrations of 0.10 and 0.15 Vac/lattice site. The FCC structure breaks down only after the vacancy concentration increases to 0.20 Vac/lattice site.

Comparison of results from MC and MD simulations for both the Al-Vac and Ni-Vac systems shows that the structures resulting from MD simulations at times of 1 ps are the same as equilibrium structures. Figure 7 shows a result for Ni-0.15 Vac/lattice site that is typical for all Al-Vac and Ni-Vac systems. The RDFs calculated based on MD and MC simulations are identical in Fig. 7.

Effect of Vacancy Distribution

The initial vacancy distribution does not affect lattice stability for most Al-Vac and Ni-Vac systems. Figure 8 compares RDFs for initial random and ordered vacancy distributions that were calculated from MD simulations of Ni containing 0.10 or 0.20 Vac/lattice site. These results show that RDFs for random and ordered vacancies are identical. This behavior is typical of most Al-Vac and Ni-Vac systems.

The exception to the above trend is the case of Ni containing 0.15 Vac/lattice site. For this case, random vacancies enhance lattice stability compared to ordered vacancies. Figure 9 shows RDFs for random and ordered vacancy distributions that were calculated from MD simulations of Ni containing 0.15 Vac/lattice site. The RDF for random vacancies shows distinct peaks at the first-nearest neighbor through fifth-nearest neighbor positions. In contrast, nearest-neighbor peaks for ordered vacancies are either diffuse or missing. These results indicate that the FCC structure is intact for random vacancies but not for ordered vacancies.

The conclusions on lattice stability for random and ordered vacancy distributions are supported by calculations of total potential energy at 0K. Figure 10 compares the energy per Ni atom vs the number of vacancies per lattice site for both random and ordered vacancy distributions. The plot shows that energy/Ni atom is identical for all systems, except for Ni-0.15

Vac/lattice site. For this case, the distribution of random vacancies has a much lower energy compared to the distribution of ordered vacancies.

Effect of Hydrogen

Hydrogen degrades the lattice structure of Al for all vacancy concentrations. Figure 11 shows RDFs calculated from MD simulations at 300K for Al containing 0.10 Vac/lattice site plus 0.5 H/Al atom as well as Al containing 0.10 Vac/lattice site without hydrogen. The RDF for Al-0.10 Vac/lattice site without H reflects some FCC structure, whereas RDF peaks are much less defined for the case with hydrogen. These results are typical for all Al-Vac systems.

The effect of H on the stability of Ni-Vac systems is more complex compared to the Al-Vac cases. Short-time MD simulations at 300K suggest that the effect of H depends on vacancy concentration. Figure 12 shows RDFs calculated for Ni lattices containing 0.10 or 0.15 Vac/lattice site without H and the same Ni-Vac systems with 0.5 or 1.0 H/Ni atom. One notable feature in Fig. 12 is that the RDF peaks for the systems with H are shifted to larger distances due to lattice expansion from the interstitial solute. The nearest neighbor peaks for the Ni-Vac systems with H are smaller and broader than the peaks for the cases without hydrogen. This indicates that the FCC structure is less defined for Ni-Vac systems containing hydrogen.

In contrast to the results for Ni-0.10 Vac/lattice site and Ni-0.15 Vac/lattice site, the lattice order for Ni containing 0.20 Vac/lattice site is improved by hydrogen. Figure 13 shows RDFs calculated from MD simulations at 300K for Ni-0.20 Vac/lattice site plus 1.0 H/Ni atom as well as Ni-0.20 Vac/lattice site without hydrogen. While neither RDF in Fig. 13 distinctly reflects the FCC structure, the nearest neighbor peaks for the distribution representing Ni-0.20 Vac/lattice site plus 1.0 H/Ni atom are better defined than for the system without hydrogen.

Equilibrium structures determined from MC simulations suggest that hydrogen disrupts lattice order for all Ni-Vac systems. Figure 14 compares RDFs calculated from MD and MC simulations of Ni-0.20 Vac/lattice site plus 1.0 H/Ni atom. The far-neighbor peaks of the RDF calculated from the MC simulation are not as well defined as those calculated from the MD simulation, suggesting that the most stable structure consists of a disordered lattice. The RDFs calculated from MC simulations for the other Ni-Vac plus H systems are identical to the RDFs calculated from MD simulations; conclusions on lattice stability can be derived from the MD results for these cases (Fig. 12).

Summary

- High vacancy concentrations cause the Al lattice to disorder at 300K. Aluminum is not a likely candidate for consideration as an atomically porous material for hydrogen storage.
- Nickel retains the FCC structure at 300K for vacancy concentrations up to 0.15 Vac/lattice site. Unexpectedly, the lattice with 0.15 Vac/lattice site is more stable than the lattice with 0.10 or 0.20 Vac/lattice site. The Ni systems with 0.10 and 0.15 Vac/lattice site exhibit domains consisting of uniform lattice rotations. The Ni lattice with 0.15 Vac/lattice site is more stable with an initial distribution of random vacancies compared to ordered vacancies.
- The equilibrium lattice structures of Ni and Al containing vacancies and H are less ordered compared to structures with vacancies only at 300K.

References

- [1] Y. Fukai and N. Okuma, "Evidence of Copious Vacancy Formation in Ni and Pd Under a High Hydrogen Pressure," *Japan Journal of Applied Physics*, vol. 32, pp. L1256-L1259, 1993.
- [2] Y. Fukai and N. Okuma, "Formation of Superabundant Vacancies in Pd Hydride Under High Hydrogen Pressures," *Physical Review Letters*, vol. 73, pp. 1640-1643, 1994.
- [3] Y. Fukai, "Formation of Superabundant Vacancies in Metal Hydrides at High Temperatures," *Journal of Alloys and Compounds*, vol. 231, pp. 35-40, 1995.
- [4] K. Nakamura and Y. Fukai, "High-Pressure Studies of High Concentration Phases of the Ti-H System," *Journal of Alloys and Compounds*, vol. 231, pp. 46-50, 1995.
- [5] K. Watanabe, N. Okuma, Y. Fukai, Y. Sakamoto, and Y. Hayashi, "Superabundant Vacancies and Enhanced Diffusion in Pd-Rh Alloys Under High Hydrogen Pressures," *Scripta Materialia*, vol. 34, pp. 551-557, 1996.
- [6] M. S. Daw and M. I. Baskes, "Embedded-Atom Method: Derivation and Application to Impurities, Surfaces, and other Defects in Metals," *Physical Review B*, vol. 29, pp. 6443, 1984.
- [7] M. S. Daw, S. M. Foiles, and M. I. Baskes, "The Embedded Atom Method: A Review of Theory and Applications," *Materials Science Reports*, vol. 9, pp. 251-310, 1993.
- [8] Y. Fukai, Y. Kurokawa, and H. Hiraoka, "Superabundant Vacancy Formation and Its Consequences in Metal-Hydrogen Alloys," *Journal of the Japan Institute of Metals*, vol. 61, pp. 663-670, 1997.
- [9] J. E. Angelo, N. R. Moody, and M. I. Baskes, "Trapping of Hydrogen to Lattice Defects in Nickel," *Modelling and Simulation in Materials Science and Engineering*, vol. 3, pp. 289-307, 1995.
- [10] M. I. Baskes, J. E. Angelo, and N. R. Moody, "Atomistic Calculations of Hydrogen Interactions with Ni₃Al Grain Boundaries and Ni/Ni₃Al Interfaces," in *Hydrogen Effects in Materials*, A. W. Thompson and N. R. Moody, Eds. Warrendale, PA: The Minerals, Metals, and Materials Society, 1996, pp. 77-90.
- [11] M. I. Baskes, X. Sha, J. E. Angelo, and N. R. Moody, "Trapping of Hydrogen to Lattice Defects in Nickel," *Modelling and Simulation in Materials Science and Engineering*, vol. 5, pp. 651-652, 1997.

Fig. 1 Radial distribution functions for the Al-Vac system after energy minimization at 0K.

Fig. 2 Radial distribution functions for the Al-Vac system calculated from MD simulation at 300K.

Fig. 3 Radial distribution functions for the Ni-Vac system after energy minimization at 0K.

Fig. 4 Energy per Ni atom vs vacancies per lattice site calculated from energy minimization at 0K.

Fig. 5 (a) Atom positions for Ni-0.15 Vac/lattice site after energy minimization at 0K. (b) Atom positions of lattice in (a) after 3° rotation around $[010]$ axis.

Fig. 6 Radial distribution functions for the Ni-Vac system calculated from MD simulation at 300K.

Fig. 7 Comparison of radial distribution functions for Ni-0.15 Vac/lattice site calculated from MD and MC simulations at 300K.

Fig. 8 Comparison of radial distribution functions for Ni-0.10 Vac/lattice site and Ni-0.20 Vac/lattice site containing either initially random or ordered vacancies at 300K.

Fig. 9 Comparison of radial distribution functions for Ni-0.15 Vac/lattice site containing initially random or ordered vacancies at 300K.

Fig. 10 Comparison of energy per Ni atom vs vacancies per lattice site for initially random or ordered vacancies at 0K.

Fig. 11 Radial distribution functions calculated from MD simulations at 300K for Al-0.10 Vac/lattice site plus 0.5 H/Al and for Al-0.10 Vac/lattice site without hydrogen.

Fig. 12 Comparison of radial distribution functions calculated from MD simulations at 300K for the Ni-0.10 Vac/lattice site and Ni-0.15 Vac/lattice site systems with and without hydrogen.

Fig. 13 Comparison of radial distribution functions calculated from MD simulations at 300K for Ni-0.20 Vac/lattice plus 1.0 H/Ni and Ni-0.20 Vac/lattice site without hydrogen.

Fig. 14 Comparison of radial distribution functions for Ni-0.20 Vac/lattice site plus 1.0 H/Ni from MD and MC simulations at 300K.

DISTRIBUTION:

- 1 U. S. Department of Energy
Office of Basic Energy Sciences
Attn: A. L. Dragoo
Washington, D.C. 20545
- 1 U. S. Department of Energy
Office of Basic Energy Sciences
Attn: Iran L. Thomas
Washington, D.C. 20545
- 1 U. S. Department of Energy
Office of Basic Energy Sciences
Attn: R. Gottschall
Washington, D.C. 20545
- 1 Abteilung für Oberflächenchemie und Katalys
Universität Ulm
Attn: R. J. Behm
Albert-Einstein-Allee 11
D-89081 Ulm/Donau
Federal Republic of Germany
- 1 Ames Laboratory
Iowa State University
221 Metals Development
Attn: J. H. Rose
Ames, IA 50011
- 1 Arizona State University
Dept. of Materials Science
Attn: J. B. Adams
Tucson, AZ 85721
- 1 Argonne National Laboratory
9700 S. Cass Avenue
Attn: D. M. Gruen
Argonne, IL 60439
- 1 Argonne National Laboratory
Materials Science Division
Bldg. 212
Attn: Dr. Dieter Wolf
9700 S. Cass Avenue
Argonne, IL 60439

- 1 Battelle Pacific Northwest
Attn: R. H. Jones
P. O. Box 999
Richland, WA 99352
- 1 Brookhaven National Laboratory
Attn: J. W. Davenport
Upton, Long Island, NY 11973
- 1 Brookhaven National Laboratory
Attn: D. Welch
Upton, Long Island, NY 11973
- 1 Brown University
Department of Physics
Attn: P. J. Estrup
Providence, RI 02912
- 1 Dr. R. Bullough
Materials Development Div.
B552 Harwell Laboratory
Oxfordshire OX11 0RA
England
- 1 California Inst. of Technology
Attn: T. C. McGill
Pasadena, CA 91125
- 1 California Inst. of Technology
Attn: T. Tombrello
Pasadena, CA 91125
- 1 Carnegie-Mellon University
Attn: P. Wynblatt
Dept of Met. Engr. and Matls. Science
3325 Science Hall
Pittsburgh, PA 15213
- 1 Cornell University
Laboratory of Atomic and Solid State Physics
Attn: N. W. Ashcroft
Ithaca, NY 14853-2508
- 1 Cornell University
Bard Hall
Attn: J. M. Blakely
Ithaca, NY 14850

- 1 Cornell University
School of Chemical Engineering
Attn: Prof. Paulette Clancy
Olin Hall
Ithaca, NY 14853-1501
- 1 Cornell University
Dept. of Materials Science and Engineering
Attn: Prof. S. L. Sass
Ithaca, NY 14853-1501
- 1 Eastman Kodak Company
Research Laboratories, Bldg. 81
Attn: Dr. J. R. Lavine
Rochester, NY 14650-2008
- 1 Eindhoven University
Attn: H. H. Brongersma
Dept. of Physics
P. O. Box 513
5600 M. B. Eindhoven
The Netherlands
- 1 Fritz-Haber Institut
Faradayweg 4-6
Attn: G. Ertl
1000 Berlin 33
Federal Republic of Germany
- 1 Fysik Institut
Odense Universitat
Attn: P. Sigmund
DK-5230 Odense M
Denmark
- 1 Georg-August-Universitat Gottingen
Institut Fur Metallphysik
Attn: Prof. Reiner Kirchheim
Hospitalstr. 3-7, D-37073 Gottingen
Germany
- 1 George Washington University
School of Engineering and Applied Science
Attn: Charles Gilmore
Associate Dean for Research
Tompkins Hall
Washington, D. C. 20052

- 1 Georgia Institute of Technology
Attn: Prof. Uzi Landman
225 North Avenue N.W.
Atlanta, GA 30332
- 1 Hahn-Meitner-Institut
Attn: H. Wollenberger
Glienicke Str. 100
1000 Berlin 39, West Germany
- 1 Harvard University
Attn: Prof. H. Ehrenreich
Cambridge, MA 02183
- 1 Harvard University
Attn: Prof. J. R. Rice
Cambridge, MA 02183
- 1 Haverford College
Department of Physics
Attn: L. Roelofs
Haverford, PA 19041
- 1 IBM
Almaden Research
K33.801
Attn: Farid F. Abraham
650 Harry Road
San Jose, CA 95120-6099
- 1 IBM
Fishkill Laboratory
Dept. 62G
Attn: Dr. Cheruvu S. Murthy
Hopewell Junction, NY 12533
- 1 IBM.
T. J. Watson Research Center
Attn: P. M. Marcus
P. O. Box 218
Yorktown Heights, NY 10598
- 1 IBM.
T. J. Watson Research Center
Attn: J. Tersoff
P. O. Box 218
Yorktown Heights, NY 10598

- 1 Institut für Festkörperforschung der Kernforschungsanlage
Attn: P. H. Dederichs
Postfach 1913
D-5170 Jülich 1, West Germany
- 1 Institut für Festkörperforschung der Kernforschungsanlage
Attn: W. Schilling
Postfach 1913
D-5170 Jülich 1, West Germany
- 1 Institut für Festkörperforschung der Kernforschungsanlage
Attn: H. Wenzl
Postfach 1913
D-52405 Jülich,
Germany
- 1 Institut für Physikalische Chemie
Freie Universität Berlin
Attn: K. Christman
Takush. 3
1000 Berlin 33
Germany
- 1 Institute of Corrosion and Protection of Metals Academia
Sinica
No. 62 Wencui Road
Shenyang 110015, China
- 1 Institute of Metal Research
Chinese Academy of Sciences
Attn: Dr. Xianwei Sha
72 Wenhua Road
Shenyang, 110015
P. R. China
- 1 Interfaculty Reactor Institute
Attn: Dr. A. van Veen
Mekelweg 15
NL-2629JB, Delft
The Netherlands
- 1 International School for
Advanced Studies
Attn: Prof. F. Ercolessi
I-34014 Trieste
Italy

- 1 International School for Advanced Studies
Attn: E. Tosatti
I-34014 Trieste
Italy
- 1 Iowa State University
Ames Laboratory
Attn: K.-M. Ho
Ames, IA 50011
- 1 Iowa State University
Ames Laboratory
Attn: P. A. Thiel
Ames, IA 50011
- 1 Professor Ryoichi Kikuchi
1702 Comstock Dr.
Walnut Creek, CA 94595-2469
- 1 Lab. Voor Fysische Metaalkunde
Materials Science Centre
Attn: J. Th. M. De Hosson
Groningen, Nijenborgh 18
The Netherlands
- 1 Lawrence Berkeley Laboratory
Materials and Molecular Res. Div.
Attn: M. L. Cohen
Berkeley, CA 94720
- 1 Lawrence Berkeley Laboratory
Materials and Molecular Res. Div.
Attn: S. G. Louie
Berkeley, CA 94720
- 1 Lawrence Berkeley Laboratory
Materials and Molecular Res. Div.
Attn: G. A. Somorjai
Berkeley, CA 94720
- 1 Lawrence Berkeley Laboratory
Attn: A. W. Thompson
One Cyclotron Road, MS 66-203
University of California
Berkeley, CA 94720

- 1 Lawrence Berkeley Laboratory
Materials and Molecular Res. Div.
Attn: M. A. van Hove
Berkeley, CA 94720
- 1 Lockheed Martin Idaho Technologies
Attn: Clint Van Siclen
P. O. Box 1625
Idaho Falls, ID 83415-2211
- 1 Los Alamos Natl. Scientific Lab.
Attn: S. P. Chen
Theoretical Div T-11 MS B262
P. O. Box 1663
Los Alamos, NM 87545
- 1 Los Alamos Natl. Scientific Lab.
Attn: Dr. Terry C. Lowe
MST-5, MS G730
P.O. Box 1663
Los Alamos, NM 87545
- 1 Los Alamos Natl. Scientific Lab.
P. O. Box 1663
Attn: A. Voter
Los Alamos, NM 87545
- 1 Loyola College
Department of Physics
Attn: Prof. R. S. Jones
4501 N. Charles St.
Baltimore, MD 21210
- 1 Lucent Technologies
Attn: M. J. Cardillo
Murray Hill, NJ 07974
- 1 Lucent Technologies
Attn: Y. C. Chabal
Murray Hill, NJ 07974
- 1 Lucent Technologies
Attn: D. R. Hamann
Murray Hill, NJ 07974

- 1 Massachusetts Inst. of Technology
 Attn: Prof. A. S. Argon
 Cambridge, MA 02139
- 1 Massachusetts Inst. of Technology
 Attn: Prof. R. M. Latanision
 Cambridge, MA 02139
- 1 Massachusetts Inst. of Technology
 Attn: S. Yip
 Cambridge, MA 02139
- 1 Max-Planck-Institut für Plasmaphysik
 Attn: R. Behrisch
 D8046 Garching, West Germany
- 1 Max-Planck-Institut für Plasmaphysik
 Attn: Professor V. Dose
 D-8046 Garching, West Germany
- 1 Max-Planck-Institut für Metallforschung
 Institut für Werkstoffwissenschaften
 Attn: Prof. Dr. Phil. H. Fischmeister
 Seestrasse 92
 7000 Stuttgart 1
 Federal Republic of Germany
- 1 Max-Planck-Institut für Stromungsforschung
 Attn: Prof. J. P. Toennies
 Bunsenstrasse 10
 D-3400 Göttingen
 Federal Republic of Germany
- 1 Michigan Technological University
 Dept. of Metallurgical Engineering
 Attn: J. K. Lee
 Houghton, MI 49931
- 1 Mitsubishi Heavy Industries, Ltd.
 Attn: Ohira Tatsuya
 Advanced Technology Research Center
 Technical Headquarters
 8-1, Sachiura 1-chome
 Kanazawa-ku, Yokohama
 236 Japan

- 1 National Institute of Standards and Technology
Attn: J. M. Rowe, 235/A106
Washington, DC 20234
- 1 National Institute of Standards and Technology
Materials Bldg., Rm. A 113
Attn: R. Thomson
Washington, DC 20234
- 1 National Research Institute for Metals
Computational Matls. Science Div.
Attn: Katsuyuki Kusunoki, Dr. Eng.
1-2-1 Sengen, Tsukuba
305. JAPAN
- 1 Naval Research Laboratory
Attn: T. Andreadis, Code 4651
Washington, DC 20375
- 1 Naval Research Laboratory
Attn: Michael J. Mehl, Code 6691
4555 Overlook Ave. SW
Washington, DC 20375-5000
- 1 Nippon Steel Corporation
Attn: Dr. Tooru Matsumiya
Advanced Materials & Technology Research Laboratories
1618 Ida. Nakahara-ku
Kawasaki 211, Japan
- 1 North Carolina State University
Attn: Dr. J. Narayan
Department of Materials and Eng.
Raleigh, NC 27607
- 1 Northwestern University
Dept. of Mat. Science & Eng.
Attn: Dr. David Seidman
2145 Sheridan Road
Evanston, IL 60201-9990
- 1 Oak Ridge National Laboratory
Bldg. 4500S, MS 6114
Box 2008
Attn: W. H. Butler
Oak Ridge, TN 37831-6114

- 1 Oak Ridge National Laboratory
P. O. Box X
Attn: H. L. Davis
Oak Ridge, TN 37830
- 1 Oak Ridge National Laboratory
P. O. Box X
Attn: J. O. Steigler
Oak Ridge, TN 37830
- 1 Oak Ridge National Laboratory
P. O. Box X
Attn: M. Stocks
Oak Ridge, TN 37830
- 1 Oak Ridge National Laboratory
Attn: M. H. Yoo
Metals and Ceramics Division
P. O. Box 2008, Bldg. 5500, MS-6376
Oak Ridge, TN 37831-6376
- 1 The Ohio State University
Division of Materials Research
Attn: S. A. Dregia
Columbus, OH 43210-1106
- 1 The Ohio State University
Attn: Prof. P. Shewmon
Dept. Matl. Sci. & Engr.
116 W. 19th Ave.
Columbus, OH 43210-1106
- 1 The Ohio State University
Physics Department
Attn: J. W. Wilkins
174 West 18th Avenue
Columbus, OH 43210-1106
- 1 Oxford University
Dept. of Metallurgy and Science of Materials
Attn: Prof. D. G. Pettifor
Parks Road
Oxford OX1 3PH
England

- 1 Oxford University
Dept. of Metallurgy and Science of Materials
Attn: Adrian Sutton
Parks Road
Oxford OX1 3PH, ENGLAND
- 1 Pennsylvania State University
Attn: Barbara J. Garrison
Department of Chemistry
State College, PA 16801
- 1 Queens University
Dept. of Physics
Attn: Prof. Malcolm Stott
Stirling Hall
Kingston, Canada K7L 3N6
- 1 Rice University
Attn: Prof. R. B. McLellan
Houston, TX 77251
- 1 Rutgers University
Dept. of Ceramics
Attn: Dr. S. H. Garofalini
P. O. Box 909
Piscataway, NJ 08854
- 1 School of Mathematics and Physics
Queen's University of Belfast
Attn: M. W. Finnis
Belfast BT7 1NN
Northern Ireland
- 1 Seagate Technology
Attn: Prof. James Angelo
8001 East Bllomington Fwy.
Bloomington, MN 55420
- 1 Staatliche Materialpruefungsanstalt (MPA)
University of Stuttgart
Pfaffenwaldring 32
Attn: Dr. S. Schmauder
Pfaffenwaldring 32
D-70569 Stuttgart, GERMANY
- 1 Stanford University
Department of Chemistry
Attn: Hans C. Anderson
Stanford, CA 94305

- 1 Stanford University
 Department of Materials Science & Engineering
 Attn: Timur Halicioglu
 Stanford, CA 94305
- 1 Stanford University
 Dept. of Chemical Engineering
 Attn: Prof. R. Madix
 Stanford, CA 94305
- 1 Stanford University
 Department of Chemistry
 Attn: Prof. R. Zare
 Stanford, CA 94305
- 1 Technical University of Denmark
 Attn: J. K. Nørskov
 Lab. f. Technical Physics
 DK-2800 Lyngby, Denmark
- 1 Ukrainian Academy of Sciences
 Attn: V. Pokropivny
 V. Ogorodnikov
 Institute for Problems of Matls. Science
 Computer Simulation Laboratory
 Ukrainian 252680 KIEV GSP-142
- 1 University of Aarhus
 Institute of Physics
 Attn: F. Besenbacher
 DK-8000 Aarhus C, Denmark
- 1 University of Aarhus
 Institute of Physics
 Attn: J. Bottiger
 Ivan Stensgaard
 DK-8000 Aarhus C, Denmark
- 1 University of California
 MANE Department
 Attn: N. M. Ghoniem
 6275 Boelter Hall
 Los Angeles, CA 90024
- 1 University of California, Berkeley
 Department of Materials Science & Mineral Engineering
 Attn: Prof. D. C. Chrzan
 577 Evans
 Berkeley, CA 94720

- 1 University of California, Irvine
Department of Physics
Attn: Prof. A. Maradudin
Irvine, CA 92717
- 1 University of California, Irvine
Department of Physics
Attn: Prof. M. Mills
Irvine, CA 92717
- 1 University of Connecticut
Center for Materials Simulation
Attn: Professor Phil Clapp
97 North Eagleville Rd.
Storrs, CT 06269-3136
- 1 University of Connecticut
Department of Metallurgy
Attn: Jonathan A. Rifkin
97 North Eagleville Rd.
U-136
Storrs, CT 06269-3136
- 1 University of Copenhagen
H. C. Ørsted Institute
Attn: H. H. Andersen
Universitetsperken 5
DK-2100 Copenhagen, Denmark
- 1 University of Illinois
Dept. of Mining and Metallurgy
Attn: H. K. Birnbaum
Urbana, IL 61801
- 1 University of Illinois
Nuclear Eng. Lab.
Attn: D. Ruzic
103 S. Goodwin Ave., Rm. 214
Urbana, IL 61801
- 1 The University of Liverpool
Dept. of Materials Science and Engineering
Attn: Prof. D. J. Bacon
P. O. Box 147
Liverpool L69 3BX, ENGLAND
- 1 University of Maryland
Department of Physics
Attn: T. Einstein
College Park, MD 20742-4111

- 1 University of Maryland
Department of Physics
Attn: Dr. K. E. Khor
College Park, MD 20742-4111
- 1 University of Michigan
Dept. of Mat. Sci. and Engr.
Attn: D. Srolovitz
Ann Arbor, MI 48109-2136
- 1 University of Michigan
Dept. of Nuclear Engineering
Attn: G. Was
Ann Arbor, MI 48109
- 1 University of Minnesota
Dept. of Chemical Engr. And Materials Science
Attn: J. R. Chelikowsky
151 Amundson Hall
421 Washington Avenue S. E.
Minneapolis, MN 55455
- 1 University of Minnesota
Corrosion Research Center
Attn: W. W. Gerberich
Minneapolis, MN 55455
- 1 University of Minnesota
Corrosion Research Center
Attn: R. A. Oriani
Minneapolis, MN 55455
- 1 University of New Mexico
Chemistry & Nuclear Eng. Dept.
Attn: Dr. Anil Prinja
Albuquerque, NM 87131
- 1 University of Pennsylvania
Department of Materials Science
Attn: V. Vitek
Philadelphia, PA 19104
- 1 University of Texas
Depts. of Astronomy & Physics
RLM 15-212
Attn: R. Smoluchowski
Austin, TX 78712

- 1 University of Trieste
Dipartimento di Fisica Teorica
Attn: Prof. N. Parrinello
I-34014 Trieste
Italy
- 1 University of Virginia
Department of Materials Science
Attn: R. A. Johnson
School of Engineering and Applied Science
Charlottesville, VA 22901
- 1 University of Wisconsin
ECE Department
Attn: Prof. W. N. G. Hitchon
Madison, WI 53706
- 1 Vanderbilt University
Dept. of Mechanical Engineering
Attn: Prof. William F. Flangan
Box 1592, Station B
Nashville, TN 37235
- 1 Virginia Commonwealth University
Dept. of Physics
Attn: Prof. P. Jena
Richmond, VA 23284-2000
- 1 Virginia Commonwealth University
Dept. of Physics
Attn: Prof. T. McMullen
Richmond, VA 23284-2000
- 1 Virginia Polytechnic Institute and University
Department of Materials Science and Eng.
Attn: Yri Mishin
Blacksburg, VA 24061
- 1 Virginia Tech
Materials Engineering Dept.
Attn: Prof. Diana Farkas
213 Holden
Blacksburg, VA 24061-0237
- 1 Washington University
Department of Physics
Campus Box 1105
Attn: Anders Carlsson
St. Louis, MO 63130

1 Washington State University
Dept. of Mechanical and Materials Engineering
Attn: Richard Hoagland
Pullman, WA 99164-2920

1 Westinghouse Savannah River Co.
Attn: Myung W. Lee
Savannah River Technology Center
Bldg. 773-42A, Room 144
Aiken, SC 29808

1 Westinghouse Savannah River Co.
Attn: Ralph Wolf
Scientific Computation Section
Bldg. 773-42A
Aiken, SC 29808

1 Westinghouse Electric Corporation
Bettis Atomic Power Laboratory
Attn: Richard W. Smith
Post Office Box 79
West Mifflin, PA 15122-0079

1 West Virginia University
Dept. of Physics
Attn: Bernard R. Cooper
Morgantown, WV 26506

1 J. W. Elmer, L-355
1 A. Gonis, L-268
1 W. E. King, L-356
1 P. E. A. Turchi, L353

1	MS 0149	D. L. Hartley, 4000
1	MS 0149	C. E. Meyers, 4000
1	MS 0161	B. W. Dodson, 11500
1	MS 0337	R. D. Skocypec, 9002
1	MS 0457	H. W. Schmitt, 2000
1	MS 0513	R. J. Eagan, 1000
1	MS 0601	J. S. Nelson, 1113
1	MS 1056	S. M. Myers, 1112
1	MS 1056	B. L. Doyle, 1111
1	MS 1056	W. R. Wampler, 1111
1	MS 1079	A. D. Romig, 1300
1	MS 1320	W. G. Perkins, 6832
1	MS 1349	T. P. Swiler, 1846
1	MS 1405	E. A. Holm, 1841
1	MS 1411	F. Yost, 1841

1	MS 1413	D. R. Jennison, 1114
1	MS 1413	G. L. Kellogg, 1114
1	MS 1413	T. A. Michalske, 1114
1	MS 1423	G. C. Osbourn, 1155
1	MS 1427	S. T. Picraux, 1100
1	MS 9001	T. O. Hunter, 8000
		Attn: J. B. Wright, 2200
		D. L. Crawford, 5200
		M. E. John, 8100
		L. A. West, 8200
		W. J. McLean, 8300
		R. C. Wayne, 8400
		P. N. Smith, 8500
		P. E. Brewer, 8600
		L. A. Hiles, 8800
		R. C. Wayne, 8900
1	MS 9052	M. Allendorf, 8361
1	MS 9108	S. L. Robinson, 8412
1	MS 9161	K. L. Wilson, 8716
1	MS 9161	M. D. Asta, 8717
1	MS 9161	S. M. Foiles, 8717
1	MS 9163	W. Bauer, 8302
1	MS 9214	C. F. Melius, 8117
50	MS 9403	M. I. Baskes, 8712
1	MS 9403	S. E. Guthrie, 8712
1	MS 9403	N. R. Moody, 8712
25	MS 9403	B. P. Somerday, 8712
1	MS 9405	T. M. Dyer, 8700
		Attn: C. M. Hartwig, 8701
		J. C. F. Wang, 8713
		G. J. Thomas, 8715
		E.-P. Chen, 8742
		P. E. Nielan, 8743
		W. A. Kawahara, 8746
1	MS 9409	G. D. Kubiak, 8250
1	MS 9409	R. H. Stulen, 8250
3	MS 9018	Central Technical Files, 8940-2
1	MS 0899	Technical Library, 4916
1	MS 9021	Technical Communications Department, 8815/ Technical Library, MS 0899, 4916
1	MS 9021	Technical Communications Department, 8815 For DOE/OSTI