Grant DE-FG06-87ER45287

SUMMARY ACCOMPLISHMENTS

Grant DE-FG06-87ER45287 was active during the period from June 1987 through May, 1998 at which time the grant identification was changed. During the period for which Grant DE-FG06-87ER45287 was active the research program was initially titled "Metal Induced Embrittlement". A somewhat different research topic was pursued under the same grant identifier but with the title "The Role of Defect Structures in Grain Boundaries on the Deformation and Fracture Behavior of Crystalline Solids" which began upon renewal of the program June 1, 1995 and continued until a second renewal occurred on June 1, 1998 under the new grant designation DE-FG03-98ER45697. Therefore this report is intended to provide a recapitulation of the achievements during the active period of Grant DE-FG06-ER45287.

The principal achievements of this work are represented by the papers published in refereed literature, the presentations at national and international symposia, and the degrees granted to students that were supported by this grant. These items are included in separate sections below. The following list highlights some of the most notable findings that derive from the research supported under Grant DE-FG06-ER45287.

- Measurements of the K-dependence of the crack growth rates in aluminum alloys in contact with liquid Hg and Ga.
- Experimental determination of the effect of strength level of aluminum alloys on the K-da/dt embrittlement response.
- Explanation of the plastic wake effect on liquid metal embrittlement (LME) phenomena.
- Measurement and explanation of the effect of oxygen on LME of aluminum alloys.
- Measurement of the temperature dependence and the activation energy for grain boundary penetration of Ga in aluminum.
- Development and implementation of techniques for performing in-situ observation and characterization of Ga penetration of grain boundaries in a TEM.
- Development of models explaining the driving force and kinetics for LME processes.
- Atomistic simulation of crack tips identifying the principal factors controlling the emission of dislocations and ductile versus brittle behavior.
- Atomistic studies that help to describe the effect of dissolved hydrogen on the competition between dislocation emission and fracture of fcc metals.
- Atomistic studies of LME.
- Atomic simulation of short-circuit diffusion within dislocation cores.
- Evaluation of the relevance of various grain boundary defects to GB fracture and sliding processes.
- The use of atomistic simulations to evaluate the strength of dislocation barriers.
- Correlation of grain boundary structure with Ga penetration velocities in general grain boundaries in aluminum.

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- Development of a methodology to characterize grain boundary structure using Ga penetration phenomena.

These topics, and others, are described in the papers, presentations, and theses identified in the next two sections.

Publications and Presentations Under Grant DE-FG06-87ER45287

1. Y. Liu and R. G. Hoagland, "Chaotic Crack Growth Behavior During LME of Aluminum", presented at the 1988 Fall Meeting of TMS, Chicago, IL, Sept. 26, 1988.

2. R. G. Hoagland, "Atomic Simulation of Crack Tips in Aluminum Using an Embedded Atom Potential", presented at the 1988 Fall Meeting of TMS, Chicago, IL, Sept. 26, 1988.

3. R. G. Hoagland, "Designing Advanced Materials", presented at WEST '88 Symposium, Seattle, WA, Oct. 17, 1988.

4. Y. Liu and R. G. Hoagland, "Transient and Intermittent Crack Growth During Embrittlement of 7075-T651 Aluminum by Mercury", Scripta Met., **23** (1989) pp 339-344.

5. B. Benson and R. G. Hoagland, "Crack Growth Behavior of a High-Strength Aluminum Alloy During LME by Gallium", Scripta Met, **23** (1989), pp. 1943-1948.

6. B. Benson and R. G. Hoagland, "Crack Growth Behavior in Aluminum Embrittled by Liquid Gallium", presented at the Annual Meeting of AIME-TMS, Phoenix, AZ, Feb., 1989.

7. R. G. Hoagland, M. S. Daw, S. M. Foiles, and M. I. Baskes, "An Atomic Model of Crack Tip Deformation in Aluminum Using an Embedded Atom Potential", J. Mater. Res., **5**,(1990) pp 313-324.

8. R. G. Hoagland, M. S. Daw, S. M. Foiles, and M. I. Baskes, "The Nature of Crack Tip Fields in Atomic Scale Models of Aluminum", in proceedings of, Atomic Scale Calculations of Structure in Materials, ed. by M. S. Daw and M. A. Schluter, MRS Vol. 193, (1990) pp. 283-288.

9. R. G. Hoagland, Y. Liu, and B. Benson, "Influence of Microstructure on Liquid Metal Embrittlement of Aluminum Alloys", in Fracture Behavior and Design of Materials Structures, Vol. 1, ed. by D. Firrao, proc. of ECF8, Turin, Italy, (1990) pp. 316-321.

10. R. G. Hoagland, M. S. Daw, and S. M. Foiles, "Some Aspects of Forces and Fields in Atomic Models of Crack Tips", presented at the Annual Meeting of AIME-TMS, 1991, New Orleans, LA. .

11. R. G. Hoagland, M. S. Daw, and J. P. Hirth, "Some Aspects of Forces and Fields in Atomic Models of Crack Tips", J. Mater. Res., **6**, (1991) pp. 2565-2577.

12. R. G. Hoagland, "Fundamental Aspects of Crack Tip Deformation in Atomic Models", presented at Annual meeting of APS, Cincinnati, OH, Mar. 1991.

13. R. G. Hoagland, "Fundamental Aspects of Forces and Fields in EAM Models of Cracks", presented at Univ. of Washington, Seattle, WA, April, 1991.

14. R. G. Hoagland, ""Influence of Microstructure on Liquid Metal Embrittlement of Aluminum Alloys", presented at INEEL, Idaho Falls, ID, August, 1991.

15. R. G. Hoagland, "Fundamental Aspects of Atomistic Models of Cracks", presented at INEEL, Idaho Falls, ID, August, 1991.

16. R. G. Hoagland and H. Heinisch, "An Atomic Simulation of the Influence of Hydrogen on the Fracture Behavior of Nickel", J. Mat. Res., 7, (1992) pp. 2080 - 2088.

17. Y. Liu and R. G. Hoagland, "A Superdislocation Model of Crack Shielding by a Plastic Wake", Scripta Mat., **27**, (1992) pp. 253 - 258.

18. R, G, Hoagland, "Effect of Hydrogen on Dislocation Emission from a Crack Tip in Nickel", Materials Theory and Modeling, ed. by J. Broughton, P. Bristowe, and J. Newsam, Materials Res. Soc., Pittsburgh, (1993), pp. 103 - 109.

19. R. G. Hoagland, "On the Energetics of Dislocation Emission from a Crack Tip in Nickel Containing Hydrogen", J. Mat. Res., 9, (1994) pp. 1805-1819.

20 R. Hugo and R. G. Hoagland, "In Situ Observation of Gallium Penetration into Aluminum Grain Boundaries", presented at the Hydrogen and Environmental Effects Symposium, TMS Annual Mtg, Feb., 1993.

21. R. G. Hoagland and Y. Liu, "Environmental Effects on Crack Tip Processes at the Atomic Level", invited paper presented at the Int'l Conf. on Fundamentals of Fracture, Urabandai, Japan, May 31-June 4, 1993, and publ. in Materials Science and Engineering, **A176**, (1994) pp. 219 - 224.

22. R. G. Hoagland, "An Atomic Simulation of the Effect of Hydrogen on Dislocation Emission from a Crack Tip in Nickel", invited paper, IUTAM Symposium on Computational Mechanics, Providence, RI, June 1993.

24. R. G. Hoagland, "Numerical Issues in the Computational Modelling of Dislocations", invited paper, Materials/Computation Workshop: Dislocation Dynamics, Arlington, VA, May 1993.

25. R. G. Hoagland and S. Sondhi, "Crystallographic Dependence of the Energetics of Dislocation Emission from a Crack Tip", invited paper. at the TMS Special Symposium on Atomistic Effects in Deformation Mechanisms, Las Vegas, Feb. 1995.

26. R. G. Hoagland, "Atomistic Modelling of the Competition Between Dislocation Emission and Crack Extension - Relevance to Environmental Assisted Cracking", in the Proceedings of the Symposium on New Techniques for Characterizing Corrosion and Stress Corrosion, ed. by R. H. Jones and D. Baer, TMS, Cleveland, 1995.

27. R. G. Hoagland, "On the Energetics of Dislocation Emission from a Crack Tip in FCC Solids", invited presentation at Los Alamos, Feb. 1996.

28. R. G. Hoagland, "Crystallographic Aspects of Dislocation Emission from a Crack Tip in an FCC Metal", Phil Mag. A, **76**, (1997) pp. 543 - 563.

29. R. C. Hugo and R. G. Hoagland, "In-Situ Observation of Aluminum Embrittlement by Liquid Gallium", Scripta Mat. **38**, (1998) pp. 523 - 529.

30. R. G. Hoagland and A. F. Voter, "Self-Diffusion within the Cores of a Dissociated Glide Dislocation in an FCC Solid", presented at the Spring APS Meeting, Kansas City, Mar. 17 - 21, 1997.

31. R. G. Hoagland, "Atomic Modelling of Critical Processes in the Nonlinear Crack Tip Zone of Crystalline Solids", invited presentation, Fall '97 TMS Meeting.

32. R. J. Kurtz, R. G. Hoagland, and J. P. Hirth, "A Computer Simulation of an Extended Dislocation Barrier in an FCC Crystal", in the Proceedings of the Symposium on Micromechanics of Advanced Materials, TMS, Cleveland, 1996.

33. R. G. Hoagland, J. P. Hirth, R. J. Kurtz, and B. Ding, "Atomistic Simulation of Grain Boundary Defects: Dislocations and Steps", invited presentation at Spring '97 MRS, San Francisco, April, 1997.

34. M. I. Baskes, R. G. Hoagland, and T. Tsuji, "An Atomistic Study of the Strength of an Extended-Dislocation Barrier", Mod. and Simul. in Mat. Sci. and Eng'g, **6**,(1998) pp. 9 – 18.

35. R. G. Hoagland, A. F. Voter, and S. M. Foiles, "Self-Diffusion within the Cores of a Dissociated Glide Dislocation in an FCC Solid", Scripta Mat., **39**, (1998) pp. 589-596.

36. R. G. Hoagland, invited participation in the CECAM/PSIK Workshop on "Ab Initio Calculations in Relation to Modelling Constitutive Relations and Fracture Toughness of Metals", Lyon, FR, Oct. 20 - 22, 1997.

37. J. P. Hirth and R. G. Hoagland, "Extrinsically Dissociated Dislocations in Simulated Aluminum", Phil. Mag., **78**, (1998) pp. 529-532.

38. R. C. Hugo and R. G. Hoagland, "Influence of Grain Boundary Misorientation on Gallium Penetration of Aluminum", presented at "Symposium on Atomic-Level Simulation of Materials: New Methods and Novel Applications: Bulk Simulations", TMS, San Antonio, TX, Feb. 1998.

39. R. G. Hoagland, S. M. Foiles, and A. F. Voter, "Atomistic Simulation of Vacancy Diffusion Within the Cores of a Dissociated Glide Dislocation in an FCC Metal", invited paper presented at Spring MRS, San Francisco, April, 1998.

Degrees Awarded Under Grant DE-FG06-87ER45287

Doctor of Philosophy in Materials Science

Student	Thesis Title	PhD Awarded
Yi Liu	Crack Growth Behavior During LME	1992
Richard Hugo	The Use of In-Situ TEM Observations of Gallium Penetration to Characterize Grain Boundary Structure	1998
Liping Ren	Penetration of Ga on Interfaces in Al/X Bimetallic Composites	2000

Master of Science in Materials Science and Engineering

Yi Liu	Crack Growth Behavior During LME of High Strength Aluminum Alloy by Mercury	1988
Bradley Benson	Liquid Metal Embrittlement of Aluminum by Gallium	1990
Richard Hugo	Observation of Gallium Penetration by TEM	1993