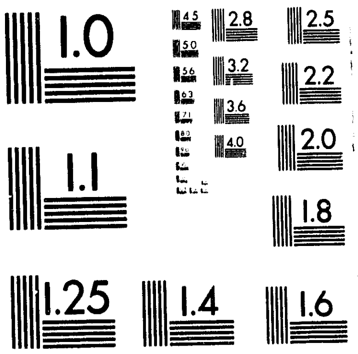
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DOE/ER/45287--3

Annual Performance Report and Planned Research

on

METAL INDUCED EMBRITTLEMENT

A Program being conducted under
DOE Grant DE-FG06-87ER45287

by

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October 1, 1990

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METAL INDUCED EMBRITTLEMENT

Summary of Progress

This section summarizes the progress made in this program from the start of the renewal on March 1, 1990, to date. The program is investigating the cause of embrittlement that results when certain solid metals and their alloys are exposed to other metals, usually in liquid form. The research is examining a number of factors that influence the degree of embrittlement and is also attempting to develop the basis for understanding the underlying cause of embrittlement. Accordingly, the program is a blend of theoretical and experimental approaches.

The experiments have largely involved crack growth experiments of aluminum embrittled by liquid mercury and gallium and progress in the current contract period has been made in the following areas:

- Plastic Wake Effects - A superdislocation model of the the plastic wake generated by a growing crack was developed to estimate the effect which the wake has on the crack tip J. The motivation stems, in part, from the very large influence of yield strength on embrittlement, with heat treatable aluminum alloys displaying a decreasing K needed to sustain crack propagation with increasing strength. The model indicates that the contribution from the plastic wake is rather modest, and so does not explain the strength effect except in the cases of most severe embrittlement where the crack growth process occurs entirely along intergranular paths at very low K levels.

- Effect of Liquid Composition - Both Ga and Hg embrittle aluminum and its alloys, but the effect of Ga is much more severe, as the K-threshold in the presence of Ga is zero (or, actually, at a negative K), whereas, the K-threshold in the presence of Hg is typically about +4 $MPa\sqrt{m}$. The addition of even small amounts of Ga to Hg, i.e. 1 at %, produces a gallium-like response. A feature that distinguishes Ga from Hg which is believed to account for this effect is that Ga is a much stronger oxide former than Hg and therefore "getters" dissolved oxygen in the liquid. Indeed, the free energy of formation of gallium oxide is larger than that of aluminum oxide, which, if allowed to form at the crack tip, inhibits the cracking process.

• Strength Effects and the F1/F2 Model - The effect of strength on the degree of embrittlement has been examined in considerable detail. One way to characterize the degree of embrittlement is to identify the K-level at which a certain crack velocity is achieved. Measurements of the susceptibility have been conducted over a broad range of strength levels in 1100, 2024 and 7075 aluminum alloys. A a further step toward explaining these results, and, indeed, the cause of embrittlement. per se, a model called F1/F2 was developed. This model considers the total force acting to extend the crack tip, F1, and the total force acting to emit dislocations from the tip, F2. Our model is a variant of the Rice-Thompson picture in which the resistance to crack extension and to dislocation emission are compared as competing processes. If dislocation emission occurs prior to crack extension, tough, ductile fracture is favored, and the reverse favors a brittle, low toughness response. Our model employs results derived from our atomistic simulation work to estimate the forces controlling dislocation emission and crack extension and their dependence on the flow strength of the solid. A comparison between the predictions of the model and the experimental results are quite favorable suggesting that most, but not all, of the major features of the mechanisms that affect Metal Induced Embrittlement are understood.

Progress in the more theoretical aspects of the program in the current contract period have derived from work involving atomic simulations of the events occurring at a crack tip as follows:

• Determination of Stresses, Strains, and Crack Tip Forces in Atomic Models - In order to relate all of the factors and events that shape the behavior and response of the crack tip in atomistic models to the behavior on more macroscopic levels, it is not only convenient but crucial that the stress and strain fields be obtainable in the atomic-scale crack tip models as they are in continuum models of cracks. Accordingly, considerable effort has been expended to devise methods for computing the stress and strain tensors at the atoms in the atomistic models in a way which is nearly consistent with their definition in continuum mechanics. Procedures for calculating the stresses and displacement gradients at each of the atom locations in arbitrarily strained lattices were developed. These procedures allow comparison of the "actual" crack tip fields in the atomistic models with the continuum predictions, e.g. the HRR field or the linear elastic field. Furthermore, the various conservation integrals, such as the forces represented by the J, M, and L-integrals are now readily calculable, and, in addition, the forces acting to cause various events at, or in the vicinity of, the crack tip, such as dislocation emission and crack extension, are now available. The principle motivation for developing these tools is to provide a quantitative means of assessing the effects of adsorbing foreign atoms near the crack tip. Some examples of some very recent results of such calculations are contained in an Appendix accompanying this report.

Personnel

This study is currently supporting one graduate student, Mr. Yi Liu who is basing his PhD dissertation on the research supported by this program. He expects to complete his work at approximately the end of 1991 or early 1992. Mr. Liu is involved in both the theoretical and experimental aspects of the program. Another graduate student, Mr. Brad Benson received his MS early in 1990, and based his research on this program. The Principal Investigator, R. G. Hoagland is directing the experimental work and is also conducting the atomistic modeling.

Other Federal Funding

DOE - ``Metal Induced Embrittlement," $365,000; 3/87-2/92.(This program)

PNL/DARPA - ``High Temperature Beryllides," $280,000; 6/89-5/92, with J.P. Hirth (PI).

Washington Technology Center - ``High Temperature Beryllides," $75,000; 6/89 - 5/92, with J.P. Hirth (PI).

NSF - "Nanoclusters", $450,000; 6/90 - 5/93, with C. T. Crowe (PI), J. Chung, C. H. Hamilton, and J. P. Hirth.

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. 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.

6. 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.

7. 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.

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, accepted for publication in proceedings of, Atomic Scale Calculations of Structure in Materials, San Francisco, CA, April, 1990.

9. R. G. Hoagland, Y. Liu, and B. Benson, Influence of Microstructure on Liquid Metal Embrittlement of Aluminum Alloys, accepted for publication in the Proceedings of Eighth International Conf. on Fracture, Turin, Italy, Oct. 1-5, 1990.

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

11. R. G. Hoagland and J. P. Hirth, Atomic Scale Stresses, Strains, and Forces at Crack Tips, to be submitted to J. Mater. Res.

Planned Research During the Second Budget Period

In general, no significant changes in the work plan, relative to that described in the Renewal Proposal for the period 3/1/90 to 2/28/92, are anticipated at this time. Work will strive to further clarify the various mechanisms involved during crack extension and to strengthen the ideas concerning the fundamental cause of the embrittlement process. Specifically, we intend to:

- complete the experimental investigation of the effect of liquid composition on embrittlement.

- examine in greater detail the differences between intergranular and transgranular (cleavage) paths. Some experiments involving intergranular crack paths in Al bicrystals are planned.

- complete the development of EAM potentials that can mimic foreign atoms introduced near the crack tip and conduct the necessary calculations to assess the consequences of the presence of such atoms on the competition between dislocation emission and crack extension.

- continue the Sandia/WSU interaction which has been so useful to the program.

Appendix: Effect of Dislocation Emission on the Crack Tip Field

The following figures show some examples of results of stress and strain calculations in EAM models of aluminum in two instances: in Figure 1 which shows a crack in a lattice subject to a stress intensity of 0.32 MPa$\sqrt{m}$, and in Figure 2 which shows the same lattice but with the K increased to 0.34 MPa$\sqrt{m}$. Therefore, this is about the stress intensity level needed to trigger plastic flow at the crack tip. The Griffith K for this material is close to 0.3 MPa$\sqrt{m}$, but, because of lattice trapping, the actual K needed to start crack advance is larger than this. The crack plane is (110) and the crack propagation direction is [111]. The actual model size is somewhat larger than shown as there are atoms around the periphery of these pictures which do not appear here.

Figures 3 and 4 show 3-D graphs plotting the distribution, in the X-Y plane, of the shear stress acting parallel to the glide plane (111) and in the direction of the Burgers vector of the partials that are emitted [112]. Figure 3 is prior to emission and Figure 4 is the distribution just after emission. The two humps in the shear stress distribution on either side of the crack plane (on $Y = 0$, $X < 0$) in Figure 4 clearly define the locations of the two partials. Note also that the peak in the glide stress prior to emission is located at the crack tip and has a value about equal to $\mu/10$. This corresponds to the theoretical shear strength of the solid relative to emission of a partial from the crack tip. Figures 5 and 6 show distributions of the dilatation component of the strain, i.e. the relative volume change expressed as $\Delta V/V$ (which is also $\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}$), for the two cracks. Again, the change in the patterns due to dislocation emission is striking. These results display a wealth of information concerning the consequences of the stress and strain reorganization the accompanies crack tip plasticity. In particular, they provide a useful alternative to continuum theory to assess the competition between flow and fracture and the relaxation that occurs at a crack tip by dislocation emission.

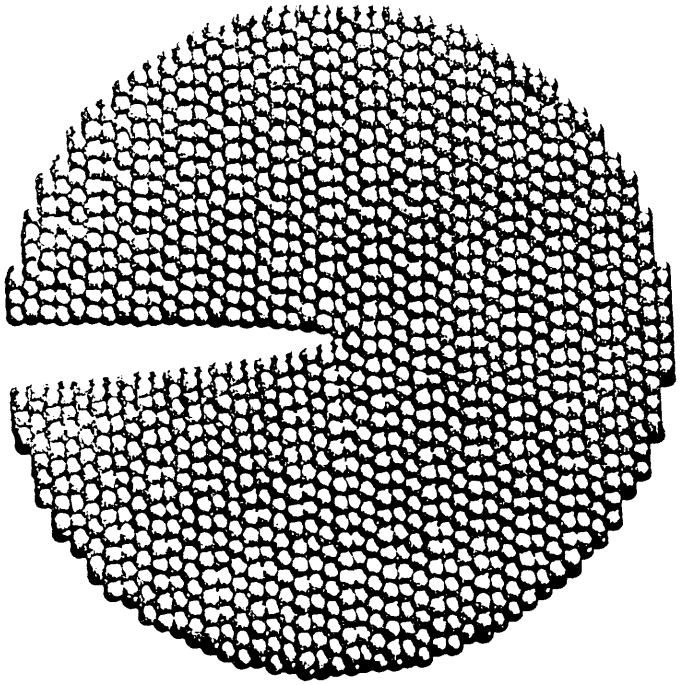

Figure 1

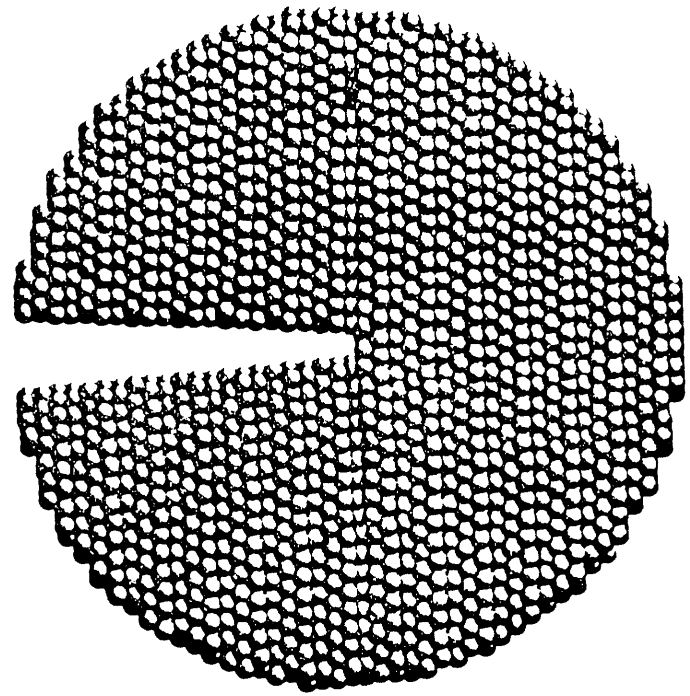

Figure 2

Figures 1 and 2. The atomic configuration of a crack in a model using an EAM potential for aluminum and loaded to a K of 0.32 MPa$\sqrt{m}$ and 0.34 MPa$\sqrt{m}$ in Figure 1 and 2, respectively, which is slightly above the Griffith K of about 0.30 MPa$\sqrt{m}$ for this material. The slight increase in K from Figure 1 to 2 has caused the emission of two partial dislocations on either side of the crack on the two [111] glide planes perpendicular to the crack plane. The consequences of the dislocation emission are noticeable by the increased CTOD that appears in Figure 2. The model diameter is 100 A and the orientation is: crack plane = (110), crack propagation direction = [111].

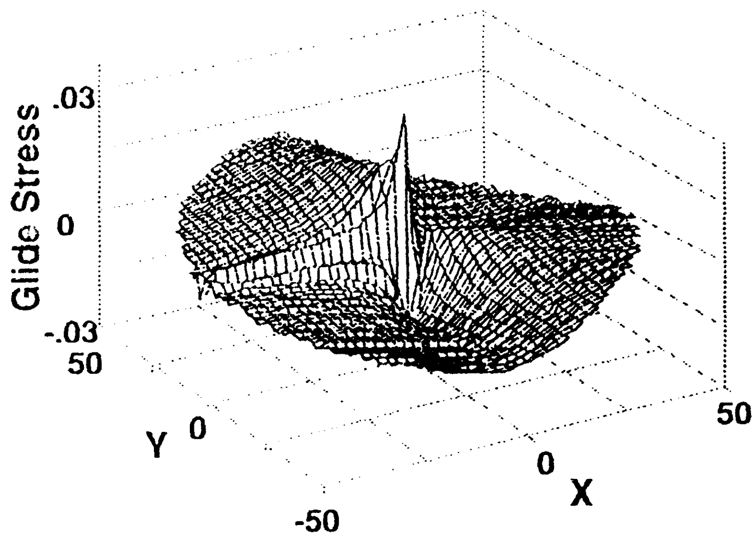

Figure 3

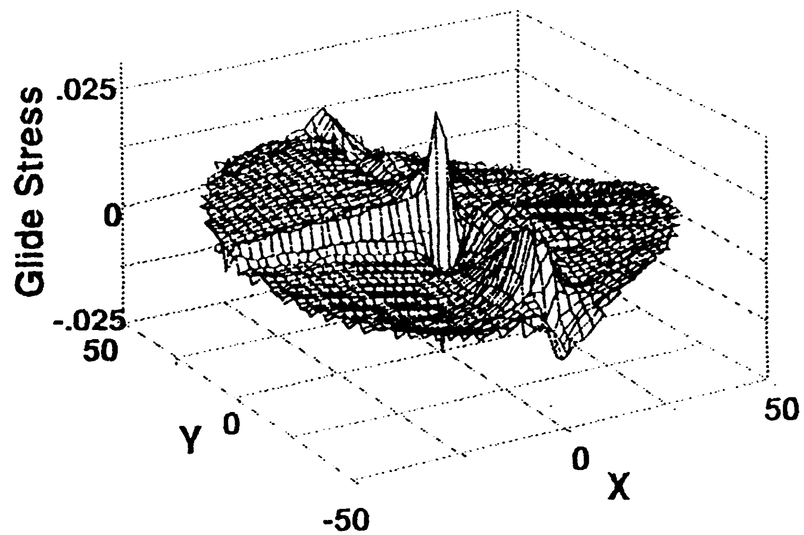

Figure 4

Figures 3 and 4. The glide component of the shear stress acting on the partials emitted in Figure 2. This glide stress is plotted in the X-Y plane where X is the direction of crack propagation and Y is perpendicular to the crack plane. Figure 3 shows the glide stress distribution prior to dislocation emission and Figure 4 after emission. Stress units are eV/A^3 and distances in A.

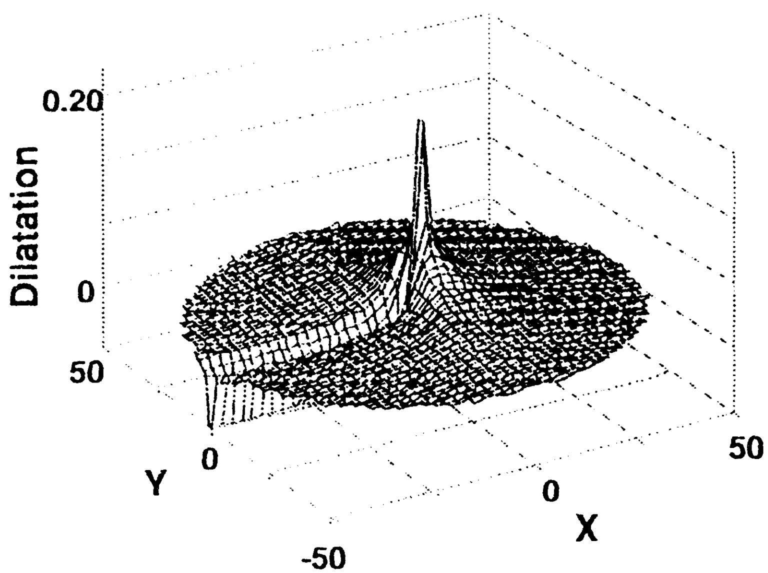

Figure 5

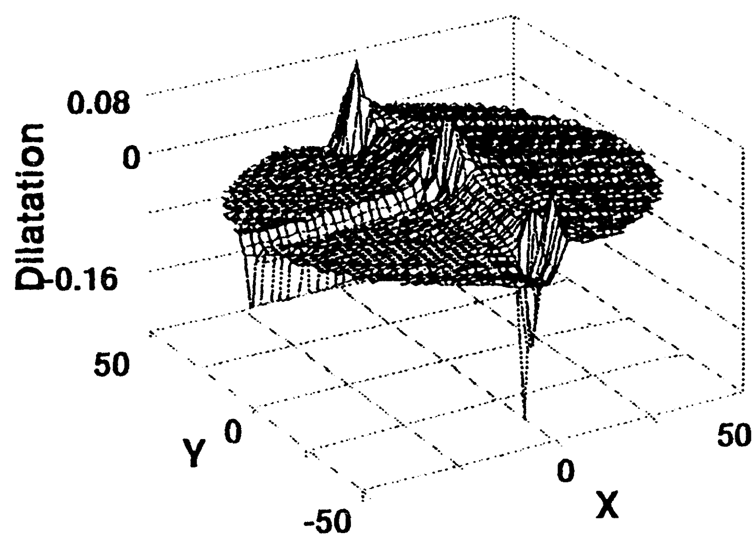

Figure 6

Figures 5 and 6. The distribution of the dilatation in the X-Y plane in the before (Figure 1) and after (Figure 2) models. The dilatation is the relative volume change ΔV/V and is computed by adding the three normal strains at each atom. X and Y refer to model coordinates, parallel to the crack plane and perpendicular to the crack plane, respectively.

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