CONTINUUM MODELING OF HYSTERESIS IN A METAL HYDRIDE SYSTEM

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Charging many metal films or powders with hydrogen results in the growth of second phase metal-hydride particles. A large volume difference between hydride and metal can induce plastic deformation and result in a significant hysteresis upon removal of the hydrogen. For a palladium hydride system (with an 11% volume change), we estimate this hysteresis with calculations of the elastic and plastic works of forward and reverse transformations using a two-dimensional finite-element model. Figure 1 shows that the results of these calculations agree quite well with experimental measurements. We also use a three-dimensional phase field model[1] that incorporates a simple model of plasticity to determine the effects of particle interactions, but for the isotropic dilation in the Pd/PdH system, these inter actions do not apparently have a significant effect. This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

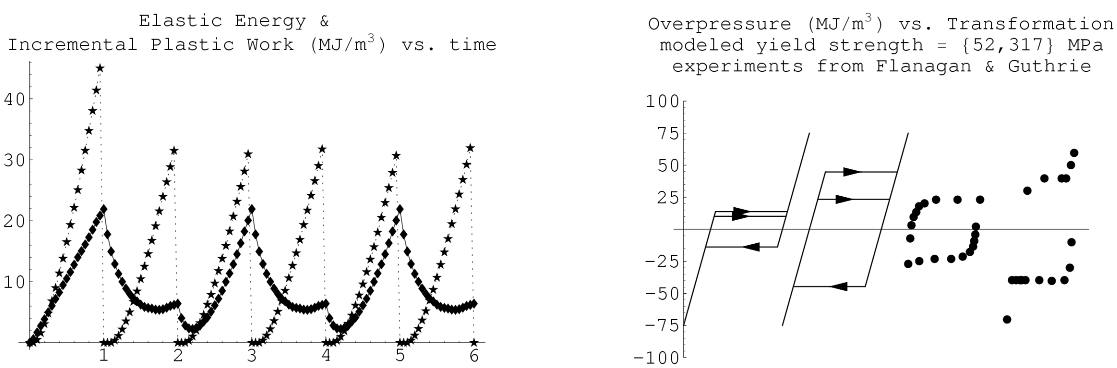

Figure 1: On the left is plotted elastic energy (stars) and plastic work (diamonds) as a palladium hydride particle expands and contracts in the lattice. In this example, the yield strength is 317 MPa and represents a fully work hardened material. On the right are predicted pressure hysteresis curves (plotted in units of chemical work) calculated for two different yield strengths and for two sets of experimental data[2,3].For an elastic-perfectly plastic material, the hysteresis is greater for the first cycle than for subsequent cycles. If the dominant source of the hysteresis is mechanical, the experimental hysteresis curves imply an effective yield strength of around 200 MPa.

References

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