PREDICTION OF THE BEHAVIOR OF STRUCTURAL MATERIALS
UNDER IRRADIATION THROUGH MODELING OF THE MICROSTRUCTURE

Progress Report
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W. G. Wolfer
University of Wisconsin
Madison, Wisconsin 53706

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Progress Summary

- 1) A general formulation was completed to derive the irradiation creep rate in single crystals. The theory allows to compute the strain rate tensor for any crystal orientation, any stress tensor, as well as for any distribution of Burgers vectors in the dislocation loop population and the dislocation network. Special cases were investigated for fcc single crystals with no preferred Burgers vector in the dislocation structure. Uniaxial tension and torsion results were presented in both analytical and graphical form. The latter results are applicable to single crystal irradiation creep tests in ion-bombardment or neutron experiments. A manuscript (Appendix A) of this work was accepted for publication in Phil. Mag.
- 2) An investigation was initiated and completed on the capture efficiencies of interstitial-type and vacancy-type loop. The objective of this research was to resolve a long-standing paradox. Previous theoretical work had shown that both types of loops should have identical capture efficiencies. Nevertheless, numerous experimental observations have revealed both types of loops. This was usually explained as due to vacancy cluster collapse of collision cascades. However, this explanation cannot explain the large interstitial-type and vacancy-type loops in zirconium alloys.

As a result of this research, it was found that non-linear elastic effects produce a significant difference in the capture efficiency such that an interstitial-type loop has a substantially larger bias than a vacancy-type loop for preferential interstitial absorption. This important result implies that vacancy loops can nucleate as well as grow during irradiation, and previous interpretations based on vacancy cluster collapse may be incorrect. Part of this work (Appendix B) has been

published in Physics Letters.

- 3) Whereas a difference in the capture efficiencies is a necessary condition for the simultaneous formation of both loop types, it is by no means a sufficient condition. This is due to the fact, that there exists an appreciable barrier for vacancy loop nucleation, but only a small one or none for interstitial loop nucleation. A nucleation theory for vacancy loops was developed, and the conditions with regard to displacement rate, irradiation temperature, and microstructure were established for vacancy-type loops to nucleate. Among other results it was found that the vacancy loop nucleation is suppressed when the capture efficiency of the entire sink structure is below a critical value. Such a situation exists when voids are present or when a high dislocation density exists.

A paper (Appendix C) ^{presented} was presented at the International Conference on Dislocation Modeling in Physical Systems.

- 4) For the nucleation of voids at temperatures larger than about half of the melting point, T_m , helium or other insoluble gases are essential. At very high helium concentrations, and at temperatures greater than $0.3 T_m$, blistering is an important mechanism for erosion. In all these problems and others involving helium, a reliable gas law is needed.

Accordingly, an equation of state for gaseous helium was developed, which can be applied regardless of the gas pressure or temperature. Comparison of the developed equation of state with experimental data gave results to within 3%. The small deviation is of the same order as the experimental error in the data.

- 5) The new equation of state for gaseous helium was applied to equilibrium gas bubbles in solids. It was found that the equilibrium bubble radius depends mainly on the number of helium atoms in the cavity, but very

little on the temperature. This is in contrast to results obtained with either the van der Waals gas law or the ideal gas law. Both gas laws, however, cannot be applied to the high helium density found in small equilibrium bubbles. The developed equation of state for helium represents therefore an important improvement.

The developed equation of state for gaseous helium was presented at the 10th ASTM International Symposium on Effects of Radiation on Materials (Appendix D). *removed*

- 6) For the explanation of blistering, two opposing models had been proposed in the past. In one theory, the gas overpressure in small cavities was thought to create stresses in the matrix which exceeded the theoretical strength of the crystal. The predictions were made with an empirical gas law extrapolated to pressures an order of magnitude larger than the experimental data. If an ideal gas law were employed in this model, the matrix stress would be less than the yield stress.

A second model, based on the lateral stresses produced in the bombarded layer, was therefore believed to be the correct explanation for blistering. However, our analysis revealed, that the lateral stresses saturate long before blistering occurs. These inconsistencies in both models, as well as which one is applicable, were resolved by using our new equation of state for helium.

It was found that the gas pressure model predicts the onset of blistering at a helium concentration which agrees with the measured ones. Furthermore, the matrix ruptures at the ultimate tensile strength rather than at the theoretical tensile strength.

Our results, presented at the 4th International Conference on Plasma Surface Interactions (see *removed* Appendix E), resolve the controversy over the

mechanism of blistering.

- 7) Impurity trapping of vacancies and/or interstitials were previously thought to enhance recombination, and thereby reduce both void formation and irradiation creep. Previous models, however, required that the impurities be both saturable and immobile. An alternate model was developed for migrating impurity atoms. It was found that fast-diffusing impurity atoms also suppress void formation. On the other hand, slow-diffusing impurity atoms enhance void formation. This appears to contradict previous explanations on the action of immobile traps. An examination of this difference revealed, however, that it arises from the assumption that a vacancy trapped at an immobile impurity atom cannot be a nucleation site for a void. Removing this restriction shows that both models predict the same result, namely, that slow-diffusion or even immobile vacancies may indeed enhance void nucleation.

A paper (^{revised} Appendix F) is in preparation for publication in Journal of Nuclear Materials.

- 8) A preliminary experiment with an eccentric pressurized tube, suspended vertically in a furnace, was carried out until earlier brittle creep rupture occurred. Subsequent measurement of the tube curvature was according to the brittle creep damage theory enunciated by Kachanov. The profile can be fitted to a circular arc, as expected, with the exception of the deflection at the end of the tube where a bulge developed. A bulge forms in conjunction with the rupture opening, whereas the uniform curvature is due to grain boundary cavitation and wedge cracks. These precede the final failure.

During the reporting period, an experimental apparatus was completed to continuously measure the tube deflection. This apparatus has been

tested with an eccentric tube in place to measure the axial temperature distribution along the tube. The distribution is uniform to within $\pm 3^{\circ}\text{C}$. The temperature varies with time by less than $\pm 1^{\circ}\text{C}$.

The elastic deflection upon pressurization of the tube was measured and found to be in agreement with theoretical predictions. Furthermore, repeated pressurizations did confirm that it is fully reversible, as it should be.

Based on all preliminary tests, the apparatus is ready for continuous measurement of the creep damage deflection.