FINAL REPORT

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**“In-Service Design & Performance
Prediction of Advanced Fusion Material
Systems by Computational Modeling and
Simulation”**

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Summary

This final report on "In-Service Design & Performance Prediction of Advanced Fusion Material Systems by Computational Modeling and Simulation" (DE-FG03-01ER54632) consists of a series of summaries of work that has been published, or presented at meetings, or both. Further details can be found in the cited references or presentations that generally can be accessed on the internet, or provided upon request to the authors. Further, it is noted that this effort was integrated with our base program in fusion materials, also funded by the DOE OFES.

1. A Transport and Fate Model for Helium and Helium Management

This work was carried out in collaboration with UC Berkeley (Wirth et al) and PNNL (Kurtz et al) to develop and apply a multiscale model of the transport and fate of helium [1-3]. One focus is to develop a model in support of microstructural design of high performance nanostructured ferritic alloys (NFAs) for fusion reactor first wall and blanket structures. Ideally, NFAs would manage very high concentrations of helium, of up to 2000 appm, while exhibiting microstructural and dimensional stability at high temperatures up to 200 dpa. Further, NFAs can be developed exhibit a good balance of mechanical properties, like high creep strength and adequate fracture toughness [4]. The key characteristics of the NFAs is that they contain nm-scale precipitates of Ti-Y-Fe-O solutes, have fine to ultra-fine crystallite grain sizes and, possibly, high dislocation densities [5-6]. To date, the model has specifically focused on intermediate to high irradiation temperatures, above the displacement damage and defect cluster dominated microstructural evolution regime. Rate theory is used to model helium transport and vacancy-helium clustering at various sites, including at dislocations, grain boundaries and coherent nanoscale precipitate interfaces. These rate theory models are supported by molecular dynamics (MD) and Monte Carlo (MC) models of key mechanisms and material parameters. Key mechanisms include substitutional and interstitial helium diffusion and their interactions with self-interstitials and self-interstitial clusters, dislocations, grain boundaries and coherent precipitate interfaces [3,7-10]. Key material parameters include the diffusion coefficients of the various migrating species, helium and vacancy binding energies with each other and with grain boundaries, dislocations/dislocation jogs and coherent interfaces. The transport model treats trapping and thermal plus ballistic de-trapping of helium at the various sites as well as self-interstitial recombination with vacancies trapped at coherent interfaces. Helium bubbles can form in the matrix, but at high temperature (e.g., 600°C) bubbles primarily form at the various trapping sites. Helium precipitation at these locations was modeled using up a simple bi-atomic nucleation plus cluster dynamics master equation growth theory.

The model was used to examine the individual and effects of the microstructural variables such as the dislocation densities, grain sizes and the nano-precipitate sizes and number densities along with the interplay of irradiation variables like temperature, dpa dose, dose rate and the He/dpa ratio. The model shows that helium can be deeply trapped in fine-scale distribution of nano-precipitate interface bubbles as well on dislocation jogs.

One example is shown in Figure 1 plotting the fractions of He collected by nano precipitates and dislocations versus grain boundaries. Notably, the grain boundaries are protected He accumulation strong trapping by nano precipitates and dislocation jogs. The model predictions will be directly compared to experimental observations primarily based on He-implanter studies on NFAs and model alloys [11-13].

Figure 1 Model prediction of the fractions of He collected by various microstructural features in a NFA as function of dislocation density.

2. Atomistic Studies of Point Defect Energetic, Dynamics and Interactions

A series of molecular statics and dynamics simulations, complemented by Lattice Monte Carlo Studies, were used to comprehensively characterize the configurations and energetics as well as the diffusion and interaction dynamics of self-interstitial atoms (SIA) and SIA clusters in Fe and simple Fe dilute Cu alloys [7,14-16]. These studies were led by researchers at LLNL, and more recently UC Berkeley, but involved active collaborations with scientists at UCSB. Among many other important results, the simulations show that SIA and SIA clusters are repelled by oversized Cu solute atoms and coherent Cu precipitates; however, SIA and SIA clusters are trapped when inside Cu precipitates. The solutes increase the three versus one-dimensional character of the diffusion of small SIA clusters. Similar studies of the energetics and dynamics of vacancies, as well as vacancy and Cu substitutional and He substitutional (He=vacancy binding) and interstitial mechanisms and diffusion coefficients were also carried out [7,9,16]. Substitutional He SIA interaction-exchange reactions leading to interstitial He were also shown to be energetically favorable [7]. Since the results of this work are well described in journal publications they will not be further detailed here.

3. Multiscale Modeling of Fracture

A Micromechanical Model of the Master Curve (MC) Universal Fracture Toughness-Temperature Curve Relation, $K_{Jc}(T - T_0)$

We have developed a suite of multiscale models in support of the highly efficient master curves-shifts method (MC- ΔT_0) method to measure and apply cleavage fracture

toughness, $K_{Jc}(T - T_o)$, data. A reference temperature, T_o , indexes the invariant master curve (MC) shape on an absolute temperature (T) scale. T_o shifts (ΔT_o) are used to account for various effects of size and geometry, loading rate and irradiation embrittlement (ΔT). The multiscale model, relating atomic to structural scale fracture processes, underpins the MC- ΔT method [17-18].

At the atomic scale, we proposed that the intrinsic micro-arrest toughness, $K_{\mu}(T)$, of the bcc ferrite solute strengthened lattice dictates an invariant shape of the macroscopic $K_{Jc}(T)$ curve [17-18]. We developed a model that shows that $K_{Jc}(T)$ is controlled by the alloy's true stress-strain (σ - ϵ) constitutive law, $\sigma(T, \epsilon)$, combined with a temperature-dependent critical local stress, $\sigma^*(T)$ and critical stressed volume, V^* . The local fracture properties, $\sigma^*(T)$ and V^* , are controlled by the coarse-scale brittle trigger particles microstructure. The V^* is governed by the number density and size/orientation distribution of the trigger particles while $K_{\mu}(T)$ depends on these temperature-independent microstructural parameters and $K_{\mu}(T)$. Finite element simulations are used to determine the critical loading conditions at $K_J = K_{Jc}$ when the σ^* and V^* local fracture criteria are met. The combined temperature dependence of $\sigma(T, \epsilon)$ and $\sigma^*(T)$ [or $K_{\mu}(T)$] control the invariant MC shape. The T_o depends on $\sigma(T, \epsilon)$, V^* and the magnitude of $\sigma^*(T)$. Increases in the magnitude of $\sigma^*(T)$ due to irradiation result in increases in T_o (ΔT_o), or irradiation embrittlement.

Fits to the universal shape of the MC, its lower shelf minimum and T_o shifts (ΔT_o) due to irradiation hardening require a $K_{\mu}(T)$ that is mildly temperature dependent above about 0 °C [17-18]. The $K_{Jc}(T)$, based on fitting the corresponding $\sigma^*(T)$, model is in good agreement with both the universal shape of the MC as well as irradiation induced ΔT_o . The ΔT_o shifts can be correlated with irradiation-induced increases in the yield stress ($\Delta\sigma_y$) and decreases in the strain-hardening rate at low strains. For minimal reductions in strain hardening, characteristic of low dose and intermediate temperature ($\approx 300^\circ\text{C}$) irradiations of pressure vessel steels, $\Delta T_o/\Delta\sigma_y \approx 0.7^\circ\text{C}/\text{dpa}$ [17]. However, at high dose ($\gg 1$ dpa), almost all alloys suffer large losses in strain hardening at irradiation temperatures below about 350°C . This effect reduces $C_o = \Delta T_o/\Delta\sigma_y$ to values of less than $0.6^\circ\text{C}/\text{dpa}$ for irradiations at $\approx 300^\circ\text{C}$; and in some cases, like for irradiations at 60°C , C_o is reduced to even lower values, perhaps associated with some degree of strain softening. Thus the $K_{Jc}(T)$ model provides a powerful tool to evaluate the

Figure 2 ΔT_o - $\Delta\sigma_y$ correlations for F82H.

effects of irradiation and other in-service sources of microstructural evolutions that can influence $\sigma(T, \epsilon)$, $\sigma^*(T)$ and V^* . Figure 2 shows the ΔT_o - $\Delta \sigma_y$ correlation for F82H at 60 and 300°C, and for Eurofer at 60°C.

The fundamental assumption underpinning the $K_{jc}(T-T_o)$ model is the temperature dependence of $K_{jc}(T)$. Thus to provide an independent verification of the MC shape model, we have designed and performed experiments to measure the micro-arrest toughness magnitude and temperature dependence in cleavage oriented iron single crystals. Indeed the experimental results quantitatively support the hypothesis and the fitted $K_{jc}(T)$, but suggest that solid solution alloying elements play an important role as well. [19-20]

An Embrittlement ΔT_o Prediction Model for the Irradiation Hardening Dominated Regime

In the irradiation hardening dominated regime below about 400°C, and in the absence of large quantities of helium, the coarse scale microstructures and the corresponding $\sigma^*(T)$ and V^* , are not effected by irradiation [17-18, 21-22]. Thus ΔT_o can be estimated from tensile, or even indentation hardness, tests. Further, ΔT_o can be modeled using a sub-model for $\Delta \sigma_y = h(T_i, dpa)$ as [22]

$$\Delta T_o(T_i, dpa) = C_o \Delta \sigma_y = C_o h(T_i, dpa)$$

Here C_o depends on the alloy to some extent, but is approximately independent of dose and temperature at more than a few dpa and at temperatures below 400°C, respectively, again assuming there are not very large quantities of helium present. We have derived $\Delta \sigma_y$ models based on fits of physically motivated equations for $h(T_i, dpa)$ fit to a large database on 9Cr tempered martensitic steels (TMS) irradiated at a wide range of temperatures and dose for both individual alloys and overall genetic alloy class trends [21-22]. Thus Equation 1 provides a good basis to estimate ΔT_o for a similar range of alloys and irradiation conditions in the hardening dominated embrittlement regime. Finally, Equation 1 can be used to estimate the ΔT_o associated with different loading rates based on a strain rate compensated temperature shift [21-22]. Figure 3 shows the predicted dpa dose dependence of ΔT_o assuming $C_o = 0.6^\circ\text{C}/\text{MPa}$, at various irradiation temperatures between 60 and 400°C.

Continued development of the model is aimed at providing a direct link

Figure 3 ΔT_o - $\sqrt{dpa}$ model predictions.

between an alloys composition and microstructure and $K_{Jc}(T)$ and T_o . Development of such micro-micromechanics models will provide a powerful tool not only to predict in-service performance, but also as a basis for alloy design and optimization. An example, of model guided alloy design and optimization is given in the next section. Finally, the hardening dominated ΔT_o MC model provides a basis to assess embrittlement (ΔT_o) that are not due to hardening alone, or even occur in the absence of hardening [18,21-22]. Such *non-hardening* embrittlement mechanisms, including very large ΔT_o caused by a combination of large $\Delta\sigma_y$ and very high levels of helium leading to reductions in the effective σ^* (and possibly V^*) and a transition to very brittle intergranular fracture. In both cases the non-hardening embrittlement is marked by increases in C_c (the Charpy impact test equivalent of C_o) to values in excess of 1. As discussed in the next section, non-hardening contributions to embrittlement are observed at lower helium levels for irradiations at temperatures greater than about 400°C and at lower temperatures (< 300°C) at helium levels greater than a threshold value of about 500 to 600 appm.

Non-hardening Irradiation Assisted Thermal and Helium Embrittlement of 8Cr Tempered Martensitic Steels: Compilation and Analysis of Existing Data

Data on irradiation hardening and embrittlement of 8-10Cr normalized and tempered martensitic steels (TMS) alloys has been compiled from the literature [18, 21-22]. Most of the embrittlement data, covering a wide range of irradiation conditions, is for sub-sized Charpy tests. As noted above, such embrittlement is dominated by an irradiation hardening mechanism below about 400°C and low to intermediate helium levels. However, the corresponding hardening-Charpy shift coefficient, $C_c = \Delta T_c / \Delta\sigma_y \approx 0.4 \pm 0.2^\circ\text{C}/\text{MPa}$ is about 50% lower than that for the fracture toughness reference temperature, T_o , with $\Delta T_o / \Delta\sigma_y \approx 0.6 \pm 0.1^\circ\text{C}/\text{MPa}$, indicating that sub-sized Charpy tests may provide *non-conservative* estimates of embrittlement [21-22]. Further, C_c increases at $T_i > 400^\circ\text{C}$, and indeed $\Delta T_c > 0$ are sometimes observed in association with $\Delta\sigma_y \leq 0$, indicative of a non-hardening embrittlement (NHE) contribution [18, 21-22]. Analysis of limited data on embrittlement due to thermal aging supports this conclusion, and we hypothesize that the NHE regime may be shifted to lower temperatures by radiation enhanced diffusion [18, 21-22].

Possible effects of helium on embrittlement for T_i between about 175°C and 400°C were also assessed based on observed trends in C_c or the equivalent for non-standard fracture tests [18, 21-22]. The available data is limited, scattered, and potentially confounded. However, collectively the database suggests that there is a minimal NHE due to helium up to a several hundred appm (< 500 appm). However, a contribution of helium to NHE appears to emerge at higher helium concentrations, estimated to be more than about 600 appm. This is accompanied by a transition from transgranular cleavage to intergranular fracture. Intergranular fracture generally occurs only at high $\Delta\sigma_y$. However, synergistic combinations of large $\Delta\sigma_y$ and severe NHE due to helium weakening of grain boundaries could lead to very large ΔT in first wall and blanket structures at fusion spectrum dose levels above 50 to 75 dpa. This has been modeled in terms of a radiation enhanced local diffusion of helium to grain boundaries resulting in their gradual weakening, and a corresponding decrease in the critical stress for brittle intergranular fracture, σ_{ig}^* , to

values below σ^* for cleavage [18, 21-22]. Figure 4 shows a preliminary model predictions for both ΔT_o and ΔT_c shifts and the added effect of dynamic loading for both fusion (10 appm He/dpa) and spallation proton (100 appm He/dpa). Note high He/dpa not only leads to very large ΔT_c (and presumably even larger ΔT_o) but the potential for low toughness at up to very high temperatures – that is elimination of the brittle to ductile transition.

Figure 4 Preliminary model predictions for both ΔT_o and ΔT_c shifts and the added effect of dynamic loading for both a) fusion environment (10 appm He/dpa) and b) spallation proton (100 appm He/dpa) irradiation.

A Model for the $K_{Jc}(T)$ of a High Strength NFA MA957

NFAs have high strength, thus they tend to have a low toughness. Further, the fracture toughness of NFAs that are hot extruded to consolidate the powders is highly anisotropic due to corresponding anisotropy of the grain structures that are elongated in the extrusion direction. Thus it is important to develop models of $K_{Jc}(T)$ to guide development of strong and tough NFAs. Thus we also modeled the temperature dependent fracture toughness, $K_{Jc}(T)$, of MA957 based on a statistically modified critical stress-critical stressed area (σ^* - A^*) local fracture criteria [23-24]. The finite element method was once again used to simulate the stress fields as a function of the applied loading K_J at different T in terms of the area (A) encompassed by a specified normal stress contour (σ). Ideally the critical stress (σ^*) is defined by the point of intersection of $A(\sigma)$ plots at various T . However, a statistically mediated range of A^* was recognized in our model, corresponding to the intrinsic distribution of K_{Jc} ; thus the point at which the $A(\sigma)$ at various T experience the maximum number of intersections was used to define σ^* . Figure 5 compares model predictions to measured K_{Jc} data. The fracture toughness of MA957 is strongly dependent on the specimen orientation. Analysis of cleavage initiation in the L-R orientation, with the highest K_{Jc} yielded the highest $\sigma^* \approx 3600$ MPa. In contrast, the σ^* for the C-L orientation, with the lowest K_{Jc} , yielded the lowest $\sigma^* \approx 2850$ MPa, while for the C-R orientation with intermediate K_{Jc} , $\sigma^* \approx 3000$ MPa. In the latter two cases, the

ligament planes contain directions parallel to the extrusion direction. The A^* for all orientations ranged from ≈ 30 to $400 \mu\text{m}^2$ and along with the σ^* is partly controlled by the distribution of cleavage initiation sites in the form of μm -scale Al_2O_3 particles aligned in the extrusion direction. The A^* - σ^* , was used to model median $K_{Jc}(T)$ and the corresponding curves at high and low fracture probabilities determined from a Weibull analysis. The model is in good agreement with previously measured K_{Jc} data, but requires a minimum median toughness $K_{\min}$ of $10 \text{ MPa}\sqrt{\text{m}}$ in the C-L orientation, which less than the standard Master Curve (MC) value of $30 \text{ MPa}\sqrt{\text{m}}$. We conclude that the low toughness in this orientation is due to intrinsic crystallographic texturing that produces low lattice toughness orientations, anisotropic elongated grains and the inclusion stringer nucleation sites.

The results support that high toughness in NFAs can be achieved by eliminating brittle trigger particles [4] to the maximum extent possible, while maintaining fine scale isotropic grain structures. Experimental verification of these concepts is planned for the near future [25].

Figure 5 Predicted $K_{Jc}(T)$ curves for the σ^* - A^* model for the median and specified fracture probability conditions for the: a) L-R; b) C-R and c) C-L orientations.

Cracked Body Size and Geometry Effects of Measured and Effective Fracture Toughness – Model Based MC and T_o Evaluations of F82H and Eurofer 97

The measured as well as the effective fracture toughness (K_{Jm} , K_{Je}) pertinent to structures, almost always depends on the size and geometry of the cracked body and is typically significantly greater than K_{Jc} . Size and geometry effects arise from both weakest link statistics, related to the volume under high stress near a crack tip, and constraint loss associated with large amounts of deformation in small specimens and shallow surface cracks. We have previously shown that very small test specimens, that suffer constraint loss as well as statistical size effects, yield non-conservatively higher values of measured cleavage fracture toughness, by factors of up to two or more, than are determined from larger standard reference 1TCT specimens with full constraint [18,26-28]. A physically based finite element σ^* - V^* micromechanical model has been developed and verified to accurately adjust the small specimen K_{Jm} data to a common, full-constraint reference size K_{Jr} [18,27-28]

In the first size effects study carried out in this program, the effects of constitutive and local fracture properties on constraint loss effects in plane strain fracture toughness tests of small specimens were evaluated. Constraint loss decreases the temperature (ΔT) at a specified toughness [26]. This downward temperature shift increases with decreasing: (a) specimen size, (b) ratio of σ^* to σ_y and (c) strain hardening rate. The toughness–temperature curve shift due to constraint loss increases with higher K_{Jm} and T_o . These results help guide the development and interpretation of small specimen fracture tests.

We next assembled a large fracture toughness database (≈ 200 data points) for the IEA heat of F82H for tests using a variety of specimen sizes [27]. A nominal ASTM E1921 master curve (MC) analysis yields a reference temperature $T_o \approx -119 \pm 3$ °C. However, as shown in Figure 6a, the measured K_{Jm} data were not well represented by a MC. Indeed T_o decreases systematically with a decreasing deformation limit M_{lim} starting at 200, which is much higher than the E1921 censoring limit of 30, indicating very large constraint loss in small specimens. The small scale yielding T_o at high M_{lim} is about -98 ± 5 °C. While, the scatter was somewhat larger than predicted, full 3D FE model-based adjustments for both constraint loss and statistical size effects, shown in Figure 6b, yielded a self-consistent set of K_{Jr} data with a MC with a very similar $T_o \approx -103$ °C.

More recently we carried out a size adjustment analysis on a toughness database that we had previously generated on a 14 mm Eurofer97 plate in the LS orientation [29-30]. The full specimen matrix, shown in Figure 7a, included specimens with 4 thicknesses from $B = 1.5$ to 98 mm and 3 widths from 3.4 to 14 mm. The measured toughness for eight specimens tested for each specimen type at -141 °C. The data, shown in Figure 7b, clearly show both statistical and constraint loss size effects. As shown in Figure 7c, statistical adjustments alone do not eliminate size effects. However, as shown in Figure 7d, after both statistical and constraint loss size adjustment the data reflect a much more self-consistent and homogeneous K_{Jr} population. A more detailed assessment shows that the data for the specimens with the smallest ligament ($b = 1.7$ mm) are somewhat over-adjusted. Excluding the latter results the T_o for the fully adjusted data for this alloy heat

and orientation is about $-110 \pm 5^\circ\text{C}$. The corresponding T_0 for the $b = 1.7$ mm data alone is about -95°C . While this deviation is not insignificant, it is at least conservative and the corresponding T_0 is far superior to evaluations that do not account for constraint loss size effects yielding a $T_0 \approx -127^\circ\text{C}$. Overall, these results suggest that constraint loss effects are smaller in Eurofer97 compared to F82H.

Figure 6 ASTM E 1921 master curve (MC) analysis for a) measured toughness data and b) CL adjusted data.

Size and Geometry Effects on the Effective Toughness of Cracked Fusion Structures

The size adjustment procedure can also be used to evaluate the stress and strain (load and displacement) conditions leading to cleavage fracture in thin-walled fusion structures with shallow surface cracks, representing conditions of large constraint loss [18]. This is important since, coupled with statistical effects of a cracked body's size, the effective strength and ductility of such structures are higher compared to those for thick sections, such as thick section pipes and pressure vessels. This means that the effects of irradiation embrittlement may be somewhat mitigated in the case of thin, surface cracked fusion structures. We used a simple example, as shown in Figure 8, to illustrate the profound implications of size-geometry effects on the fracture of fusion structures. This assessment is based on a metric of strength and ductility, specified as the ratios of the critical load and displacement at fracture to the corresponding yield load and displacement, P_c/P_y and Δ_c/Δ_y , respectively. Even in cases where the material experiences very brittle elastic fracture in standard tests, or in heavy/thick sections, with $P_c/P_y < 1$, the extrinsic size and geometry factors pertinent to fusion structures (small shallow cracks in thin sections, etc.) lead to $P_c/P_y > 1$ and $\Delta_c/\Delta_y \gg 1$. Indeed, we showed that in some, perhaps common, circumstances, the benefits of irradiation due to increases in P_c could more than offset the liabilities of the decreases in Δ_c .

Figure 7 A size adjustment analysis of Eurfore 97 fracture toughness data: a) the specimen matrix; b) the measured; c) statistical effect adjusted, and d) statistical and constraint loss effects adjusted data

Figure 8. P/P_y versus Δ/Δ_y showing the Δ_c/Δ_y for cleavage (red) and ductile (blue) fracture as a function of W for various crack configurations and strain hardening (sh) rates.

4. Modeling the Multiscale Mechanics of Flow Localization-Ductility Loss in Irradiation Damaged BCC Alloys

Understanding deformation and constitutive behavior in these alloys following irradiation to higher doses at low-to-intermediate temperature pertinent to fusion applications (and lower doses at low temperature) is an enormous challenge for a number of reasons. First, tensile tests often result in almost immediate necking and a nearly complete loss of uniform strain capacity. Hence true-stress strain laws cannot be directly derived from load-displacement data. Further, in this regime materials often (but not always), undergo severe internal flow localization that, in the limit, is concentrated in narrow highly strained channels surrounded by a larger volume of mildly strained material. Flow localization is very widely observed in many irradiated metals and alloys. It is typically associated with a stochastically initiated region of strain softening due to progressive destruction obstacles to slip by a sequence of penetrating dislocations. However, even in the case of the most studied material, copper, it is neither understood nor experimentally well characterized. Understanding and modeling of the causes and consequences of flow localization must include the effects of various factors such as irradiation temperature and dose (and the resulting defect features), the pattern of the evolution of flow channels as a function of strain, the effects of stress-state, and strain rate and test temperature and so on. So while it is universally agreed that flow localization occurs, there is a significant controversy as to its causes and consequences.

We have taken an approach to deformation and constitutive behavior that emphasizes the critical importance of the laws of both continuum and dislocation mechanics to model processes that are dominant on the mesoscopic and continuum scales [31]. We showed the loss of uniform strain was the result of macroscopic flow instabilities leading to necking. Both increases in the yield stress as well as reductions in strain hardening result in decreases uniform strains; and, notably, flow localization is not a necessary ingredient in immediate necking in tensile tests. We then developed a 3-D finite element procedure to derive the true-stress, true-strain constitutive laws from tensile tests by iterative simulations of load-displacement curves to the point of self-consistency. An example is shown in Figure 9. These models were coupled to an innovative technique to compare the corresponding 3-D finite element large geometry change simulations to quantitative 3-D in-situ confocal microscopy measurements of both in-plane thinning and lateral of necking for tensile tests in an optical loading stage. These studies have provided a great deal of insight on deformation of irradiated materials in the presence of flow localization. First, they showed that irradiation hardening persists up to high strains; and what even in cases showing a small initial strain softening, the material subsequently undergoes a small but finite strain hardening. Further, we showed the effects of irradiation on flow stability in a tensile test are primarily manifested in the reduction of uniform strains and acceleration of the initiation of necking. There is remarkably little effect of irradiation on the subsequent evolution of the geometry of the necked region, even in cases where there is an enormous increase in yield stress and severe flow localization.

Figure 9 a) FEA derived self-consistent true stress-strain curves of irradiated F82H and comparisons of FEA vs. experiments for the irradiations to b) 10 dpa at 200 °C, c) 3 dpa at 250 °C and d) 8 dpa at 300 °C.

We also carried out extensive finite element studies of heterogeneous deformation to better understand the mesoscopic consequences of flow localization to effective true stress-strain behavior [31]. The studies involved deformation cell simulations of an interconnected array of shear bands subject to various strain softening laws embedded in a matrix with a variable strain hardening capacity. An example is shown in Figure 10. We showed that only by imposing continuum mechanics laws can the interplay between intrinsic properties and microscopic deformation patterns be better understood. For example, this approach is clearly needed to address the obvious question: *if the shear bands are greatly softened by the passage of dislocations, then why does the bulk material remain so effectively strong?* Parametric studies of the effects of the topology and volume fractions of the shear bands, matrix and shear band constitutive laws and stress state where characterized in terms of their effects on the simulation cell-level effective stress-strain response as well as strain distributions. We showed that micromechanically and microstructurally motivated constitutive laws for the matrix and shear bands reproduced many of the features observed in the experimentally derived true stress-strain relations. Perhaps most importantly these simulations provide guidance to

experimental studies regarding various observables and their interrelations that can help to bridge the enormous gap between snapshot pictures of flow localized microstructures and robust and useful mechanics models.

Figure 10 An example of deformation cell simulations of an interconnected array of shear bands with strain softening embedded in a matrix with strain hardening.

From a practical point of view, the primary result was that J_2 incremental flow theory and empirically derivable constitutive laws can be used in finite element models to describe many (but perhaps not all) cases large deformation plasticity even in irradiated alloys experiencing severe flow localization. However, while the method was successful, we recognized that the constitutive and plasticity laws derived from tensile tests may not be fully unique and applicable to the entire range of deformation conditions of interest. Thus he has generalized the approach to measuring load-displacement curves and characterizing large geometry change deformation patterns and strain distributions to a wide variety of other test geometries to access high strains (suppress flow instabilities characteristic of a tensile test) and bound key structural conditions. These test geometries include compression cylinders, smooth, cracked and notched bend bars and modified tensile specimens with notches and holes and indentation tests. Input true-stress-strain constitutive and plasticity laws are again iteratively adjusted in finite element simulations of all these tests to obtain a maximum self-consistency with measurements of the load displacement curves and large geometry changes. While semi-empirical, this approach provides a critical element in multiscale modeling of deformation and fracture. All of these specimen configurations have been included in the US-Japan irradiation experiments on martensitic and vanadium alloys in the HFIR reactor. The resulting database will provide, for the first time, a systematic, quantitative and comprehensive foundation for finite element simulations of irradiated materials that experience severe flow localization.

5. A Universal Relation Between Indentation Hardness and True Stress-Strain Constitutive Behavior

A new and powerful indentation hardness (H) approach to evaluating the true stress (σ)-true plastic strain (ϵ), constitutive behavior of materials is described [32-33]. Since measurements of H intrinsically probe a wide-range of ϵ (up to ≈ 0.5), accurate assessment of the corresponding yield (σ_y) stress and strain hardening [$\sigma_{sh}(\epsilon)$] pose a significant challenge. Extensive elastic-plastic finite element (FE) simulations have been carried out to assess the relation between H and $\sigma(\epsilon)$. The simulations were based on both a wide variety of analytical $\sigma(\epsilon)$ relations, in the form of $\sigma(\epsilon) = \sigma_y + \sigma_{sh}(\epsilon)$, as well as actual $\sigma(\epsilon)$ derived from data on a large number of alloys with a very wide range of constitutive behavior. The analysis led to derivation of a remarkable *universal relation* between H and $\sigma(\epsilon)$ given by $H \approx 4.05(1 + 34.6 \sigma_{flow}/E)\sigma_{flow}$, where $\sigma_{flow} = \sigma_y + \langle \sigma_{sh} \rangle$, and $\langle \sigma_{sh} \rangle$ is the average strain hardening between $\epsilon = 0$ and 10%, and E is the elastic modulus. Note we use consistent MKS units of MPa for both H and σ_{flow} . The expression for $H(\sigma_{flow})$ also can be inverted to one describing $\sigma_{flow}(H)$. As shown in Figure 11, experimental σ_{flow} - H data pairs based on this definition of σ_{flow} for the large set of alloys noted above with a very diverse range of $\sigma(\epsilon)$ are in excellent agreement with the model predictions. The σ_{flow} - H relation provides insight into the large variation of the H/σ_y ratios that are observed for different materials, as well as the corresponding variation in the $\Delta H/\Delta \sigma_y$ used to estimate the $\Delta \sigma_y$ due to irradiation based on measurements of ΔH . Applications of the H/σ_{flow} relation, include both evaluating $\langle \sigma_{sh} \rangle$ in materials that have very low uniform strain capacity in standard tensile tests and measuring at $\sigma(\epsilon)$ high ϵ .

Figure 11 Experimental σ_{flow} - H correlations for tensile – hardness data pairs compared with model prediction.

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