An Investigation into Plastic Deformation of Irradiated Tungsten Microstructure at Elevated Temperatures using the Anand's Viscoplastic Model

Jonathan Marsh, You sung Han, Devendra Verma, Vikas Tomar*

School of Aeronautics and Astronautics, Purdue University, West Lafayette, IN 47907, USA

*Corresponding Author, Email: tomar@purdue.edu, Tel: 001-765-494-3423

ABSTRACT

Tensile deformation of a tungsten (W) microstructure is examined at elevated temperatures and at varying levels of irradiation. The computational framework used in this study is based on the finite element (FE) method using the Anand viscoplastic model. In order to account for viscoplasticity at high temperatures, the relevant material parameters of the Anand viscoplastic model have been determined through uniaxial tests upon W samples containing a high level of neutron irradiation. Analyses show that the effect of thermal softening decreases with increase in irradiation dose. In addition, a sigmoidal dependence of irradiation dose on the yield strength of W microstructures is observed. The FE analyses also suggest that the yield strength of W is directly correlated with temperature and irradiation dose. Based on the simulation results, an empirical relation for predicting the yield strength of W is proposed based upon the temperature and irradiation dose. The developed relation is found to predict the yield strength of W well over a wide range of temperatures and irradiation doses.

Keywords: Irradiation, B. Polycrystalline material, B. Viscoplastic material, A. Thermomechanical processes, C. Finite elements

1. INTRODUCTION

Tungsten is a leading candidate material for plasma facing components (i.e. first wall, blanket, and divertor) of the nuclear fusion reactor because of its favorable thermal and mechanical properties. The plasma facing components are exposed to a high level of neutron irradiation (approximately, 8×10^{14} n/cm²s) and are subjected to irradiation damage up to 120 dpa (displacements per atom) during the lifetime of a nuclear power plant [1]. Thus, it is important to understand the strength of W as a function of microstructure when subjected to high levels of irradiation, as well as high temperature.

High temperature and intense neutron irradiation in a nuclear reactor environment lead to microstructural changes and degradation of material properties. High-energy neutron particles collide with the neighboring atoms and a sequential set of atomic collision events occur. Such displacement cascade leads atoms to be permanently displaced from their original lattice site, forming defects. Helium (He) atoms generated from the D-T (Deuterium-Tritium) nuclear fusion reaction induce embrittlement and swelling of materials for nuclear reactors. Because of its low solubility, He atoms have a strong tendency to precipitate in vacancy sites and produce He/vacancy clusters. With an increase of temperature, He/vacancy clusters are further aggregated and lead to a decrease in ductility, reduced creep strength, and increased swelling [2]. At elevated temperature, viscoplastic behaviors become dominant, which are associated with temperature and rate-dependent deformation, leading to strain hardening and stress relaxation [3].

A range of work have been performed to develop a constitutive model for deformation behavior at high temperatures. Some of the recent studies include the model proposed by Vincent et al. [4, 5] for the mixing of two different size voids under different pressures in the irradiated material filled with fission gases. Analytical predictions for the effective flow surface and the dilation rate in the matrix was analyzed and then full-field simulations were

performed to compare the solutions. Lei et al. [6] developed an elastic-viscoplastic constitutive model for machining processes with consideration of the effect of strain rate, strain hardening, and temperature. Clayton [7] presented a constitutive framework for the description of thermo-elastic viscoplastic deformation of a single crystal. Increase in the yield strength was predicted by plasticity model developed by Krasnikov et al.[8] to describe high rate deformation of metals at high temperatures. Which was further used to calculate shear stress at different dislocation velocities and temperatures in Al-Cu alloy by Yanilkin et al.[9]. Effect of irradiation damage and crystal size on the mechanical behavior of the FCC single crystal was also explored by Xiao et al.[10]. This study founds the similar results as present in the current study with the prediction of critical crystal size for different hardening mechanisms. The yield strength of materials with irradiation dose has been investigated by several researcher including McMurtrey et al. [11] on irradiated stainless steel, Soler et al.[12] on LiF single crystal micropillars and effect of He irradiation on Cu films by Li et al.[13]. These studies reported the microstructural evolution and hardening mechanism dependence at different doses of irradiation. In the current study, effect of both temperature and irradiation dose is investigated which is further verified by experiment results from literature. More recently El-Atwani [14] and Ferroni [15] have investigated microstructure morphology changes in W due to ion irradiation. El-Atwani investigated the response of ultra-fine W surfaces exposed to low flux and fluence He ion irradiation at high temperature (600°C). El-Atwani observed that bubble formation and coalescence is not sufficient for surface damage and that a diffusion mechanism is also likely present. Large asperities were also observed, thought to be caused by bubble bursting. Ferroni observed the effect of annealing on ion irradiated W microstructures. Ferroni observed that dislocation loops forming in W increased in size and decreased in density with increasing temperature. Loop hopping was observed at temperatures as low as 300°C, increasing in frequency at 500°C,

1
2
3
4
5 and forming chains and clusters at 800°C. The same trend of increasing void size and
6
7 decreasing void density with increased temperature was also observed. Significant work has
8
9 been devoted to studying the effect of ion irradiation on materials, but very few works,
10
11 especially in the past thirty years have studied the influence of neutron irradiation, which is of
12
13 primary concern in design of materials for use in a nuclear reactor environment. Additionally,
14
15 there are no available works observing the influence of neutron irradiation on W
16
17 microstructures. Ion irradiation is instead used to simulate the effect of neutron irradiation
18
19 due to several favorable characteristics which are further detailed later in this article.
20
21
22
23

24
25 In this work, thermal softening, strain dependence of flow stresses, and thermo-elastic
26
27 coupling were considered for modeling the dynamic response of polycrystalline W-Ni-Fe
28
29 alloy. Andrade-Campos et al. [16] successfully implemented a non-linear, viscoplastic
30
31 constitutive formulation into finite element codes for the simulation of large deformation
32
33 processes at high temperature. The large deformation kinetic model was derived based on the
34
35 additive decomposition of the transformation gradient and the strain rate tensor. Busso et al.
36
37 [17] proposed a viscoplastic model to represent the deformation of solder for applications in
38
39 electronic packaging. The Baushinger effect and the stress-dependence on activation energy
40
41 are taken into account in this model. Foulk and coworkers [18] implemented a cohesive zone
42
43 formation into the nonlinear finite element algorithm with an account of elastic, elasto-
44
45 plastic, viscoplastic, and viscoelastic deformations.
46
47
48

49
50 Among such constitutive models for mechanical deformation at high temperature, the
51
52 Anand viscoplastic model [19, 20] is used in the present study, in order to study deformation
53
54 behavior of W at elevated temperatures and at varying levels of irradiation. The Anand model
55
56 has been widely used in literature for several reasons. First, no explicit yield condition and no
57
58 loading/unloading criterion are required for the use of this model. Second, the model employs
59
60
61
62
63
64
65

only one internal state variable (i.e. s) which represents the averaged isotropic deformation resistance to macroscopic plastic flow [21]. In addition, the commercial finite element code, ABAQUS/Standard offers Anand's model by way of a user subroutine. Finally, the Anand model for description of elastic-viscoplastic deformation has been validated by several previous works [21-24]). In order to employ the Anand model, material parameters should be determined from uniaxial tensile/compression tests with constant temperatures and strain rates. The objective of this work is to investigate the deformation behavior of irradiated W microstructure, using the Anand model, under the influence of varying irradiation levels and at different temperatures. In order to account for irradiation-induced damage, material parameters of the Anand model have been obtained based on literature available uniaxial tensile tests of W, irradiated by high levels of neutron irradiation with fluences of 0.4 and 0.9 $\times 10^{22}$ n/cm² ($E > 0.1$ MeV). An empirical relation of the yield strength with temperature and irradiation dose is also derived. Discussions regarding the W deformation behavior, stress/strain responses, and yield failure at the elevated temperatures under influence of irradiation are presented.

2. MATERIAL AND METHODS

2.1. Material Properties of the Grains and Grain Boundary

In the present study, three different irradiated microstructures are considered, each with different irradiation doses (i.e. 4.6 dpa, 14.9 dpa, and 22.5 dpa), as well as a single unirradiated microstructure. The plastic properties of the W grains for each model, as shown in Table 1 are taken from the work of Maloy and coworkers [25]. Maloy and coworkers [25] studied the mechanical behavior of tungsten when subjected to ion irradiation doses ranging between 0 and 23.3 dpa at room temperature and 475°C. Not only does this work provide stress-strain curves for these various irradiation doses, but also yield strength, as a function of dpa, which allows us to use interpolation to derive intermediate temperature data points (i.e.

temperatures 433 – 500 K in Table 1). The elastic properties of the W grains, as shown in Table 2 in the case of the unirradiated microstructure are derived from the work of Smid and coworkers [26].

The elastic and plastic properties of the W grain boundaries, as shown in Tables 6 and 7, respectively, are derived from the work of Han [27]. In this work, ab initio simulations were used to determine the tensile properties of W nanostructures using the Car-Parrinello method within the density functional theory framework. The nanostructures considered included variations with and without helium (He) point defects, so tensile strength and elastic properties could be determined based on the influence of irradiation. The single GB determined in these studies is used in each irradiated microstructure variant. High temperature viscoplastic deformation is modeled based on Anand's model described in the next section. The model is developed based on experiments by Steichen [29] as described in sections 2.3 and 2.4.

2.2. The Anand Constitutive Model

Anand and coworkers formulated a set of constitutive equations for large, isotropic elastic-viscoplastic deformations at high temperatures [19, 20]. In the Anand model, an internal state variable, denoted by s , with the dimension of stress, is introduced to represent the resistance to isotropic plastic flow. The internal state variable characterizes the isotropic strengthening mechanism such as dislocation density, solid solution hardening, and grain size effects, which depend on temperature and rate-dependent strain history [24]. The assumed relation between equivalent stress σ and the internal state variable s is

$$\sigma = cs, \quad c < 1 \quad (1)$$

where c is a material parameter, which is defined as

$$c = \frac{1}{\xi} \sinh^{-1} \left\{ \left[\frac{\dot{\epsilon}^p}{A} \exp\left(\frac{Q}{RT}\right) \right]^m \right\} \quad (2)$$

where $\dot{\epsilon}^p$ is the inelastic strain rate; ξ is the multiplier of stress, A is the pre-exponential factor, Q is the activation energy, T is the absolute temperature, R is the gas constant, and m is the strain rate sensitivity. From the combination of Eq. (1) and Eq. (2), the inelastic strain rate is expressed as the following

$$\dot{\epsilon}^p = A \exp\left(-\frac{Q}{RT}\right) \left[\sinh\left(\xi \frac{\bar{\sigma}}{s}\right) \right]^{1/m}. \quad (3)$$

The internal variable s is assumed to be in the following functional form

$$\dot{s} = h(\sigma, s, T) \dot{\epsilon}^p \quad (4)$$

where $h(\sigma, s, T)$ is a hardening function, associated with dynamic strain hardening and recovery processes. The evolution equation of the internal variable can be expressed as follows

$$\dot{s} = \left[h_0 \left| 1 - \frac{s}{s^*} \right|^a \operatorname{sign}\left(1 - \frac{s}{s^*}\right) \right] \dot{\epsilon}^p \quad a > 1, \quad (5)$$

where

$$s^* = \hat{s} \left[\frac{\dot{\epsilon}^p}{A} \exp\left(\frac{Q}{RT}\right) \right]^n, \quad (6)$$

where s^* is a saturation value of s corresponding to a given temperature and strain rate. h_0 and a are material parameters representing strain hardening and s is the deformation resistance. From Eq. (1), Eq. (2), and Eq. (6), along with $\sigma^* = cs^*$, one obtains

$$\sigma^* = \frac{\hat{s}}{\xi} \left[\frac{\dot{\epsilon}^p}{A} \exp\left(\frac{Q}{RT}\right) \right]^n \sinh^{-1} \left\{ \frac{\dot{\epsilon}^p}{A} \exp\left(\frac{Q}{RT}\right) \right\}^m \quad (7)$$

For a condition such that the system is isothermal and $s^* > s$, Eq. (1) and Eq. (5) give

$$\frac{d\sigma}{d\varepsilon^p} = ch_0 \left| 1 - \frac{\sigma}{\sigma^*} \right|^a \text{sign} \left(1 - \frac{\sigma}{\sigma^*} \right) \quad (8)$$

Finally, the integration of Eq. (8) gives

$$\sigma = \sigma^* - \left[(\sigma^* - cs_0)^{(1-a)} + (a-1) \{ ch_0 (\sigma^*)^{-a} \} \varepsilon^p \right]^{1/(1-a)} \quad (9)$$

Chen et al. [28] proposed a modified Anand model to improve the accuracy of the original Anand model, especially for material behaviors at small strain and relatively low temperatures. In their model, the initial deformation resistance is defined as a function of temperature, as follows

$$s_0 = S_1 + S_2 T + S_3 T^2 \quad (10)$$

and the hardening parameter h_0 is a function of temperature

$$h_0 = A_0 + A_1 T + A_3 T^2 \quad (11)$$

In the present study, Eq. (10) and Eq. (11) are used for determination of s_0 and h_0 . For the above Anand constitutive model, nine material parameters A , Q , ξ , m , $\hat{s}$, n , h_0 , a , and s_0 should be determined from experimental data at several temperatures and strain rates.

2.3. Determination of Anand Model Parameters

Material parameters of Anand's model can be determined from uniaxial tensile/compressive tests under constant temperatures and strain rates. Details of the determination procedure are as follows:

(1) The values of A , Q , m , n , and $\xi/\hat{s}$ in Eq. (7) are determined from a non-linear least square fitting.

(2) The combined material constants ch_0 , cs_0 , and a in Eq. (9) are determined from the constant strain rate data by a least square fit. The value of a is determined as the average of the values obtained from each individual test. After a is determined, the least square fitting of Eq. (9) is performed again to obtain the final value of ch_0 and cs_0 .

(3) From the values A , Q , and m obtained above, the value of the parameter ξ is determined such that the material constant c in Eq. (2) is less than unity for each test.

(4) From steps (1) - (3), c can be obtained from Eq. (2), then h_0 and s_0 are determined from step (2) at different temperatures. The constants in Eq. (10) and (11) are determined from the values of h_0 and s_0 determined at each temperature using a least squares fitting.

(5) From step (1) and (3), $\hat{s}$ is determined.

In order to determine the material parameters of the Anand model, uniaxial test data of W specimens, subjected to each irradiation dose are needed as a function of constant temperature and strain rate. However, uniaxial test data of irradiated W specimens are very rare. The authors of this article were only able to find one literature source [29] available which presents a set of uniaxial test data that enables one to determine the material parameters of the Anand model. Since this is the only available scientific report which presents test data of unirradiated and irradiated W specimens, two sets of Anand viscoplastic material parameters for unirradiated and irradiated W have been obtained based on these test results and are summarized in Table 3 through Table 5. Since this experiment was performed under the highest level of irradiation among the reported literature, one can expect that simulation results in the present study can serve as a reference value for design of plasma facing components of fusion reactors.

The determined material parameters of the Anand model based on this experimental data were tested under constant temperature and strain rates for validation. The values of saturated stress obtained from Anand's model are compared with experimental measurements performed by Steichen [29]. For comparison, temperatures ranging from $T = 473$ to 1170 K, at a constant strain rate ($\dot{\epsilon} = 0.0003$), and strain rates, ranging from 2×10^{-5} to $1 \times 10^{-1} \text{ sec}^{-1}$ and from 4.2×10^{-4} to $6.5 \times 10^{-2} \text{ sec}^{-1}$ at constant temperature for unirradiated and irradiated W were chosen, respectively. As shown in Fig. 1, the result from the Anand model and the

1
2
3
4
5 experimental measurements are in a good agreement. The model prediction overestimates the
6
7 saturation stress most by 70MPa at $\dot{\epsilon} = 0.0003$ and $T = 1170$ K, in the case of irradiated W.
8
9

10 **2.4. Use of Experimental Data**

11
12 The plastic material properties of unirradiated and irradiated W are taken from the work of
13
14 Maloy and coworkers [25], for which ion irradiated samples have been considered. Maloy
15
16 and coworkers [25] studied the mechanical behavior of tungsten when subjected to ion
17
18 irradiation doses ranging between 0 and 23.3 dpa at room temperature and 475°C. Not only
19
20 does this work provide stress-strain curves for these various irradiation doses, but also yield
21
22 strength, as a function of dpa, which allows us to use interpolation to derive intermediate
23
24 temperature data points (i.e. temperatures 433 – 500 K in Table 1). The elastic properties of
25
26 the W grains, as shown in Table 2 in the case of the unirradiated microstructure are derived
27
28 from the work of Smid and coworkers [26].
29
30
31

32
33 Steichen [29] performed uniaxial tensile tests of W, with neutron irradiation fluences of
34
35 0.4 and 0.9×10^{22} n/cm² ($E > 0.1$ MeV and $\sim 5 - 9$ dpa), [30], and compared the test results
36
37 with ones obtained from unirradiated W. Uniaxial tests were performed to determine yield
38
39 strength, ultimate strength, and total elongation at temperatures ranging from 232 °C to 871
40
41 °C and strain rates ranging from $3(10)^{-5}$ to $3(10)^{-2}$. The authors of this article were only able
42
43 to find one literature source [29] available which presents a set of uniaxial test data that
44
45 enables one to determine the material parameters of the Anand model. Therefore, the Anand
46
47 viscoplastic parameters for the models have been determined based on the work of Steichen.
48
49
50 As shown in the last section, the resulting model parameters reproduce experimental results.
51
52

53
54 The plastic properties of the grain, as derived from the work of Maloy pertain to samples
55
56 of the following irradiation doses: 0 dpa, 4.6 dpa, 14.9 dpa, and 22.5 dpa. The viscoplastic
57
58 properties of the grain, as derived from the work of Steichen [29] pertain to samples of
59
60 irradiation doses ranging between approximately 5 and 9 dpa. While ideally, the properties
61
62
63
64
65

would be derived from experiments with the exact same conditions (irradiation type, dpa, fluence, temperature, microstructure etc.), considering the available materials, we can obtain a reasonable approximation of the plastic deformation behavior of irradiated W microstructures. Additionally, since the model considered is a small slice of the actual surface of the W microstructure (through-thickness) in each case, the differing effects that arise due to ion and neutron irradiation are minimized.

2.5. Finite Element Analyses

In the present study, finite element (FE) simulations were performed using the commercial FE code, ABAQUS to study tensile deformation behavior of polycrystalline W microstructures at elevated temperatures and under the influence of irradiation. Ran and coworkers [31] performed microscopic analysis on the evolution of the microstructure morphology of W surfaces, irradiated with different Ga⁺ ion irradiation fluences ranged from 1.56×10^{17} ions/cm² to 4.7×10^{18} ions/cm², and compared them with the unirradiated W microstructure surfaces through SEM imaging. It is from these SEM images that the solid models utilized in the present study are derived. Figure 2 shows FE models of the polycrystalline W microstructures which are constructed based on such changes in morphology. The authors of this study propose that simply studying the mechanical properties of a material subjected to irradiation is not sufficient, without also accounting for the evolution of the microstructure throughout these levels of irradiation. Figure 2(a) though 2(d) show the FE models and mesh summary of unirradiated W, irradiated W (stage1), irradiated W (stage2), irradiated W (stage3), respectively. The stages 1 (S1), 2 (S2), and 3 (S3) correspond to the irradiation dose, with S1 corresponding to a dose of 4.6 dpa and S3 corresponding to a dose of 22.5 dpa. For each irradiation dose, five different temperatures, ranged from 350 K to 750 K with an increment of 100 K, were analyzed. ABAQUS offers the Anand viscoplastic constitutive model by way of user subroutine, CREEP. Material

parameters of the Anand model are determined for irradiated and unirradiated W and used to describe the viscoplastic material behaviors, along with the user subroutine CREEP.

The dimensions of each FE model are 19 μm , 19 μm , and 1 μm in x, y, and z direction, respectively. The thickness of the grain boundary (GB) is modeled as 2 μm . In reality W GBs have been shown to be of the order of few nm. However, computational analyses of Han and Tomar (2013) and experimental measurements by Kalidindi and Vachhani (2014) have shown that the effective influence of GB is over a larger material volume. In that sense, the current work models GBs as “interphase” rather than an “interface”. Interface is a sharp boundary, while interphase includes region of influence of interface up to the extent when mechanical property values start approaching grain level values. While actual determination of such size is not possible, this work assigns the thickness to have at least 4 finite elements across. The convergence analyses made sure that the GB property influence is independent of the number of elements in GB. In order to maintain an acceptable aspect ratio of FE elements as well as a feasible computational time, the GB and the sections of the grain in the vicinity of the GB are modeled with a fine mesh whereas the grain interior is modeled with a coarse mesh. The W microstructures in Fig. 2 are modeled with about 100,000 hexagonal 3D elements, the eight nodes and reduced integration (3CD8R) element type, and 11 elements in the thickness direction. The number of elements were chosen and validated through the use of a convergence test, as shown later.

2.6. A Discussion on the Choice of Material Parameters

No effort has been made to ensure that the microstructure and mechanical properties were consistent among various irradiation experiments. Generally speaking, ion and neutron irradiation effect materials in different ways. Ion irradiation tends to effect the surface primarily, while neutrons are able to penetrate much deeper into the sample and effect the bulk of the material [32]. Neutron irradiation experiments typically require 1 – 3 years of

exposure to reach appreciable fluences, while ion irradiation experiments require only tens of hours to reach 1 – 10 dpa. For these reasons, neutron irradiation experiments with the properties of interest to the current study are quite scarce. Due to this limitation, a combination of properties obtained from experiments using both ion and neutron irradiation have been utilized in this study.

3. RESULTS

3.1. Boundary Conditions and Convergence Test

Tensile loading is applied in the y-direction by imposing a displacement boundary condition along the upper and the lower surface of the specimen in Fig. 2. The displacement condition along the upper surface of each model was given as $u = 1.90 \mu\text{m}$, to produce 10% strain and the bottom surface at a rate of 0.01 s^{-1} of the specimen is constrained in the x, y, and z directions. For each simulation, five different temperatures, ranged from 350 K to 750 K with increments of 100 K, were taken into account.

In order to avoid the solution dependence on element size, convergence tests were performed with an increasing number of elements both in the thickness direction (i.e. z-direction) and in the vicinity of the GB. The specimens are modeled with five, seven, and nine elements in thickness direction, corresponding to about 28000, 38000, and 48000 total elements. In addition, in order to have a reference value for comparison, one specimen is modeled with a total of 121,000 elements and 11 elements in the thickness direction, as well as a finer mesh density in the vicinity of GB. The same boundary conditions present in the simulation were used for the convergence tests and the von Mises stress at the indicated location (Element A as shown in Fig. 3) is examined, as a function of mesh elements. Figure 3 shows that the solution approaches convergence with an increase in the number of elements and reach a convergent numerical solution when the number of elements is greater than

48,000. Based on this convergence test, the FE specimens are modeled with 11 elements in the thickness direction and about 100,000 elements in total, as indicated in Fig. 2.

3.2. Material Properties

As discussed earlier, together with the unirradiated case, three different levels of irradiation doses (i.e. 4.6 dpa, 14.9 dpa, and 22.5 dpa) are taken into account and each of irradiation doses are classified as stage 1(S1), stage 2(S2), and stage 3(S3) irradiation. Each of the W microstructure models consist of a GB and grains.

The focus of the present work is understanding influence of irradiation and microstructure on the deformation behavior of W. Although plastic deformation in irradiated materials occurs frequently through dislocation channels [33, 34], dislocations are not considered. The primary reason for this is the lack of consideration for grain boundary properties and temperature effects in models that encompass dislocation effects [8, 35]. While this is a limitation of the present work, it is necessary to study these effects.

Ab initio simulation results of Σ 31W GB are used to determine the mechanical properties of the GB [27], for input into the simulation. In the work by Han, ab initio simulations were used to determine the tensile properties of W nanostructures using the Car-Parrinello method within the density functional theory framework. The nanostructures considered included variations with and without helium (He) point defects, so tensile strength could be determined based on the influence of irradiation. Quantum mechanical simulation data is used to separate the influence of dislocation propagation that occurs during classical MD simulations from GB strength. The GB type chosen is the most occurring one found in polycrystalline W. While other GB types could also be chosen, in the absence of experiments such choice would be arbitrary. Therefore, the GB type is fixed as the one most commonly found. Future analyses will focus on the statistical influence of the variation in GB type.

Experimental data for the mechanical properties of W grains, determined through uniaxial tests of unirradiated and irradiated W, as a function of irradiation dose [25, 26, 29, 36] are used as further input for the simulation. Material properties of the GB and grains used for the present study are summarized in Tables 1, 2, 6, and 7.

FEM Results

Uniaxial tensile simulations were performed using the FE method to investigate the effect of temperature and irradiation on deformation behaviors of W microstructures. Twenty sets of temperature and irradiation conditions that include four different irradiation doses and five different temperatures were analyzed. The von-Mises stress distribution throughout the W microstructures and von-Mises stress vs strain, at the element A (shown earlier in Fig. 3) are examined for each stage of irradiation and temperature conditions. The element A is chosen for the investigation due to the following reasons: (1) as shown in Figs. 4 to 7, a high level of stress is applied in the vicinity of the GB and due to the significant difference in mechanical properties between the grain and GB, this is the most likely location of failure; (2) the location of the investigation site should be at the center of the model to make the effect of displacement boundary condition applied on the upper and lower surface negligible; (3) despite the microstructure morphology of the models changing drastically depending on the level of irradiation, this location remains in close proximity to the GB, while also remaining part of the grain. Figures 4 through 7 show the stress distribution of the W microstructures and von-Mises stress-strain relationship at element A, as a function of temperature and irradiation dose.

As shown in Figs. 4 to 7, the stress applied throughout the microstructures decreases with an increase in temperature, as a general trend under the same loading condition. It is shown that the dependence of temperature on plastic deformation decreases with an increase in irradiation dose. The temperature increase from $T = 350$ K to $T = 750$ K leads to a decrease in

1
2
3
4
5 flow stress by 2.3 times (in the case of unirradiated W) through 1.5 times (in the case of
6
7 irradiated W (stage 3)), depending on the level of irradiation doses. It is interesting to note
8
9 that different from the unirradiated W, a saturation stress is observed in the stress-strain
10
11 curves of irradiated W. In particular, a saturation stress is notably observed as temperature
12
13 and irradiation dose increase, suggesting the plastic deformation behaviors have been
14
15 influenced by such factors. The effects of irradiation dose and temperature on yield stress of
16
17 W will be examined in the next section.
18
19
20

21 **3.3. Effect of Temperature and Irradiation on Yield Strength of Tungsten**

22

23 The FE analyses show that the yield strength of W microstructures is directly affected by
24
25 the influence of temperature and irradiation dose. In this section, this result is examined. First,
26
27 the values of yield strength calculated from the present study are compared with experimental
28
29 measurements. Maloy and coworkers [25] irradiated W samples by up to an irradiation dose
30
31 of 23.3 dpa and then performed uniaxial tests at room temperature and at $T = 750$ K to
32
33 measure yield strength as a function of temperature and irradiation dose. Such experimental
34
35 results are compared with the present study in Fig. 8. As shown, the FE calculations are in
36
37 good agreement with the experimental results. Overall, the yield strength decreases as the
38
39 temperature increases for all examined irradiation doses. It is worth noting that in the case of
40
41 low irradiation dose (less than 5 dpa) the yield strength rapidly increases with irradiation dose,
42
43 while the rate of increase of yield strength with irradiation dose decreases, in the case of
44
45 moderate irradiation doses. When an irradiation dose becomes greater than 20 dpa, the
46
47 irradiation dependence of yield strength becomes negligible and the yield strength has a
48
49 saturated value as shown in Fig. 8. Such trend can be also observed in other irradiated
50
51 materials [37-40]. This phenomenon can be explained by irradiation-induced defects and its
52
53 effect on dislocation propagation. The number of defects such as vacancies and interstitials
54
55 formed by irradiation increases proportionally with irradiation dose and the defect clusters are
56
57
58
59
60
61
62
63
64
65

formed at the initial stage of irradiation. Such irradiation-induced defect clusters act as an obstacle to dislocation propagation, leading to irradiation hardening. However, as the irradiation dose increases and the density of defects in the material increases, the formation of defects is hindered by the already existing ones and the number of defects formed during an increment of irradiation dose decreases.

Analyses so far suggest that yield strength of irradiated W is directly correlated with temperature and irradiation dose. Based on the simulation results, a relation is proposed to determine the yield strength, as a function of temperature and irradiation dose. To derive the relation, it is assumed that the yield strength is calculated by the sum of the two functions

$$\sigma_y = \sigma_{ur} + \sigma_{ir} \quad (12)$$

where σ_{ur} is the yield strength of unirradiated W and σ_{ir} accounts for the irradiation-induced hardening. Zerilli and Armstrong proposed [41] the following equation to predict the flow stress of unirradiated body-centered cubic crystalline metals as a function of temperature, strain $\mathcal{E}$, and strain rate $\dot{\mathcal{E}}$

$$\sigma_{ur} = C_1 e^{(-C_2 T + C_3 T \ln \dot{\mathcal{E}})} + C_4 + C_5 \mathcal{E}^n + k d^{-1/2} \quad (13)$$

where C_1 to C_5 , n , and k are material parameters to be determined and d is the grain size. If the information on grain size is not available, the grain size term is usually incorporated into the C_4 parameter as shown in Eq. (14). Since both C_4 and the grain size term are independent of temperature, strain, and strain rate, such approach is reasonable and chosen in several works [42-44].

$$\sigma_{ur} = C_1 e^{(-C_2 T + C_3 T \ln \dot{\mathcal{E}})} + C_4 + C_5 \mathcal{E}^n \quad (14)$$

In Eq. (14), the first term accounts for the effects of thermal softening and strain-rate hardening, while the parameters C_5 and n consider strain hardening [45].

In the present study, the Zerilli and Armstrong (Z&A) equation (i.e. Eq. (14)) is used to determine the yield strength of unirradiated W. Lennon and Ramesh [42] performed uniaxial tests of unirradiated W over a wide range of temperatures and strain rates and determined the material parameters of the Z&A model based on these experiments. As mentioned earlier, the parameter C_4 in Eq. (14) is independent of temperature, strain, and strain rate. In this work, C_4 was determined using the curve fitting based on the simulation results. The comparison between the present study and the previous result [42] on the Z&A model parameters for unirradiated W is summarized in Table 8. Figure 9(a) shows the comparison between the simulation results and curve-fitting of the yield strength of unirradiated W, σ_{ur} .

The next step of analyses focuses on the derivation of the irradiation-induced hardening function, σ_{ir} in Eq. (12) based on the findings of the sigmoidal dependence of irradiation dose on the yield strength of W microstructures. Note that in Fig. (8) yield strength rapidly increases with irradiation dose at the regime of low irradiation dose (less than 5 dpa). After this region, the yield strength continues to increase with irradiation dose, but does so at a slower, decreasing rate. Finally, at the high irradiation dose, which is greater than 20 dpa, the irradiation dependence of yield strength becomes negligible and the yield strength reaches a saturated value. It is worth noting that in Fig. (8), experimental data at 300 K is compared with simulations at 350 K. Certain limitations were placed upon the simulation based on the material properties documented in literature, and thus, a simulation range of 350 K to 750 K had to be chosen. Regardless, the simulated result is in good agreement with the experimental result. Based on these observations, σ_{ir} was set to the form of an exponential function as follows

$$\sigma_{ir} = A(1 - \exp(-B\phi))^p \quad (15)$$

where ϕ is irradiation dose and A , B , and p are parameters to be determined. It is worth noting that σ_{ir} in Eq. (15) will be zero at $\phi = 0$ and will saturate to a constant value of A when the irradiation dose is sufficiently high. Using the non-linear least square method, the parameters A , B , and p were determined as $A = 774.16$ MPa, $B = 0.1285$, and $p = 0.5347$. The yield strength relation proposed in the present study is described as

$$\sigma_y = \sigma_{ur} + \sigma_{ir} = C_1 e^{(-C_2 T + C_3 T \ln \dot{\epsilon})} + C_4 + C_5 \epsilon^n + A(1 - \exp(-B\phi))^p \quad (16)$$

The parameters in Eq. (16) are presented in Table 9. The predicted values from the proposed relation of yield strength of W samples at temperatures of $T = 350$ K and $T = 750$ K are compared with the simulation results and plotted in Fig. (9). These results are also summarized in Table 10 along with the ones at temperatures of $T = 450$ K, 550 K, and 650 K. As shown, the prediction from the proposed relation is in good agreement overall with the simulation results. The proposed relation overestimates the yield strength of W by 183 MPa at $T=350$ K and 0.0 dpa, while it underestimates the yield strength by 162 MPa at $T = 450$ K and 14.9 dpa. These two points provide the greatest deviation from the general trend captured by the relation in Eq. (16).

4. CONCLUSION

In this work, FE simulations of uniaxial tensile deformation were performed to study mechanical deformation behaviors of W microstructures under the influence of irradiation and high temperature using the Anand viscoplastic model. In order to account for viscoplasticity at high temperature, the material parameters of the Anand model have been determined from uniaxial tests of W samples under varying amounts of neutron irradiation. Analyses show that the effect of thermal softening decreases with irradiation dose. In addition, the yield strength of W samples rapidly increases with irradiation dose at the regime of low irradiation (less than 5 dpa), while the rate of increase in yield strength gradually

1
2
3
4
5 decreases with irradiation dose as higher irradiation is applied to the samples. When an
6
7 irradiation dose becomes greater than 20 dpa, the yield strength reaches a saturated value.
8
9 This phenomenon is explained by irradiation-induced defects and its effect on dislocation
10 movement.
11
12
13

14 The FE analyses suggest that the yield strength of irradiated W microstructures are
15 directly correlated with temperature and irradiation dose. Changes in microstructure (grain
16 growth) ultimately had a minor effect on the plastic deformation behavior of W. Based on the
17 simulation results, an empirical equation to predict yield strength of W, as a function of
18 temperature and irradiation dose is proposed. The proposed relation consists of two terms
19 which account for both the yield strength of unirradiated W and irradiation-induced
20 hardening. The developed relation is found to predict the yield strength of W over a wide
21 range of temperature and irradiation dose. This relation will be useful to provide a guideline
22 for predicting yield strength for nuclear material applications.
23
24
25
26
27
28
29
30
31
32
33

34 **Acknowledgements**

35
36 Authors acknowledge support from US Department of Energy's Nuclear Energy University
37 Program Grant-DE-NE0000696.
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60
61
62
63
64
65

REFERENCES

- [1]. Duffy, D.M., "Fusion power: a challenge for materials science". *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 2010. **368**(1923): p. 3315-3328.
- [2]. Maria, S., "Multiscale Modelling: the role of helium in iron". *Materials Today*, 2009. **12**(11): p. 46-53.
- [3]. Wang, G.Z., Cheng, Z.N., Becker, K., and Wilde, J., "Applying Anand Model to Represent the Viscoplastic Deformation Behavior of Solder Alloys". *Journal of Electronic Packaging*, 2001. **123**(3): p. 247-253.
- [4]. Vincent, P.-G., Suquet, P., Monerie, Y., and Moulinec, H., "Effective flow surface of porous materials with two populations of voids under internal pressure: I. A GTN model". *International Journal of Plasticity*, 2014. **56**(0): p. 45-73.
- [5]. Vincent, P.-G., Suquet, P., Monerie, Y., and Moulinec, H., "Effective flow surface of porous materials with two populations of voids under internal pressure: II. Full-field simulations". *International Journal of Plasticity*, 2014. **56**(0): p. 74-98.
- [6]. Lei, S., Shin, Y.C., and Incropera, F.P., "Thermo-mechanical modeling of orthogonal machining process by finite element analysis". *International Journal of Machine Tools and Manufacture*, 1999. **39**(5): p. 731-750.
- [7]. J.D, C., "Dynamic plasticity and fracture in high density polycrystals: constitutive modeling and numerical simulation". *Journal of the Mechanics and Physics of Solids*, 2005. **53**(2): p. 261-301.
- [8]. Krasnikov, V.S., Mayer, A.E., and Yalovets, A.P., "Dislocation based high-rate plasticity model and its application to plate-impact and ultra short electron irradiation simulations". *International Journal of Plasticity*, 2011. **27**(8): p. 1294-1308.

- [9]. Yanilkin, A.V., Krasnikov, V.S., Kuksin, A.Y., and Mayer, A.E., "Dynamics and kinetics of dislocations in Al and Al–Cu alloy under dynamic loading". *International Journal of Plasticity*, 2014. **55**(0): p. 94-107.
- [10]. Xiao, X., Song, D., Xue, J., Chu, H., and Duan, H., "A size-dependent tensorial plasticity model for FCC single crystal with irradiation". *International Journal of Plasticity*, 2015. **65**(0): p. 152-167.
- [11]. McMurtrey, M.D., Was, G.S., Cui, B., Robertson, I., Smith, L., and Farkas, D., "Strain localization at dislocation channel–grain boundary intersections in irradiated stainless steel". *International Journal of Plasticity*, 2014. **56**(0): p. 219-231.
- [12]. Soler, R., Molina-Aldareguia, J.M., Segurado, J., Llorca, J., Merino, R.I., and Orera, V.M., "Micropillar compression of LiF [1×1] single crystals: Effect of size, ion irradiation and misorientation". *International Journal of Plasticity*, 2012. **36**(0): p. 50-63.
- [13]. Li, N., Nastasi, M., and Misra, A., "Defect structures and hardening mechanisms in high dose helium ion implanted Cu and Cu/Nb multilayer thin films". *International Journal of Plasticity*, 2012. **32–33**(0): p. 1-16.
- [14]. El-Atwani, O., Gonderman, S., Suslov, S., Efe, M., De Temmerman, G., Morgan, T., Bystrov, K., Hattar, K., and Allain, J.P., "Early stage damage of ultrafine-grained tungsten materials exposed to low energy helium ion irradiation". *Fusion Engineering and Design*, 2015. **93**(0): p. 9-14.
- [15]. Ferroni, F., Yi, X., Arakawa, K., Fitzgerald, S.P., Edmondson, P.D., and Roberts, S.G., "High temperature annealing of ion irradiated tungsten". *Acta Materialia*, 2015. **90**(0): p. 380-393.

- [16]. Andrade-Campos, A., Menezes, L.F., and Teixeira-Dias, F., "Numerical analysis of large deformation processes at elevated temperatures". *Computer Methods in Applied Mechanics and Engineering*, 2006. **195**(33-36): p. 3947-3959.
- [17]. Busso, E.P., Kitano, M., and Kumazawa, T., "A Visco-Plastic Constitutive Model for 60/40 Tin-Lead Solder Used in IC Package Joints". *Journal of Engineering Materials and Technology*, 1992. **114**(3): p. 331-337.
- [18]. Foulk, J.W., Allen, D.H., and Helms, K.L.E., "Formulation of a three-dimensional cohesive zone model for application to a finite element algorithm". *Computer Methods in Applied Mechanics and Engineering*, 2000. **183**(1-2): p. 51-66.
- [19]. Brown, S.B., Kim, K.H., and Anand, L., "An internal variable constitutive model for hot working of metals". *International Journal of Plasticity*, 1989. **5**(2): p. 95-130.
- [20]. Anand, L., "Constitutive Equations for the Rate-Dependent Deformation of Metals at Elevated Temperatures". *Journal of Engineering Materials and Technology*, 1982. **104**(1): p. 12-17.
- [21]. Otiaba, K.C., Bhatti, R.S., Ekere, N.N., Mallik, S., and Ekpu, M., "Finite element analysis of the effect of silver content for Sn–Ag–Cu alloy compositions on thermal cycling reliability of solder die attach". *Engineering Failure Analysis*, 2013. **28**(0): p. 192-207.
- [22]. Lin, Y.C., Chen, X., Liu, X., and Lu, G.-Q., "Effect of substrate flexibility on solder joint reliability. Part II: finite element modeling". *Microelectronics Reliability*, 2005. **45**(1): p. 143-154.
- [23]. Yu, D.-j., Chen, X., Chen, G., Lu, G.-q., and Wang, Z.-q., "Applying Anand model to low-temperature sintered nanoscale silver paste chip attachment". *Materials & Design*, 2009. **30**(10): p. 4574-4579.

- [24]. Liang, Z., Songbai, X., Lili, G., Guang, Z., Zhong, S., Yan, C., and Shenglin, Y., "Determination of Anand parameters for SnAgCuCe solder". *Modelling and Simulation in Materials Science and Engineering*, 2009. **17**(7): p. 075014.
- [25]. Maloy, S.A., James, M.R., Sommer Jr, W., Willcutt Jr, G.J., Lopez, M., Romero, T.J., and Toloczko, M.B., "The effect of 800 MeV proton irradiation on the mechanical properties of tungsten at room temperature and at 475°C". *Journal of Nuclear Materials*, 2005. **343**(1–3): p. 219-226.
- [26]. Smid, I., Akiba, M., Vieider, G., and Plöchl, L., "Development of tungsten armor and bonding to copper for plasma-interactive components". *Journal of Nuclear Materials*, 1998. **258–263, Part 1**(0): p. 160-172.
- [27]. Han, Y.S. and Tomar, V., "An ab initio study of the peak tensile strength of tungsten with an account of helium point defects". *International Journal of Plasticity*, 2013. **48**(0): p. 54-71.
- [28]. Chen, X., Chen, G., and Sakane, M., "Prediction of stress-strain relationship with an improved Anand constitutive Model For lead-free solder Sn-3.5Ag". *IEEE TRANSACTIONS ON COMPONENTS AND PACKAGING TECHNOLOGIES*, 2005. **28**(1): p. 111-116.
- [29]. Steichen, J.M., "Tensile properties of neutron irradiated TZM and tungsten". *Journal of Nuclear Materials*, 1976. **60**(1): p. 13-19.
- [30]. Davis, J.W., Barabash, V.R., Makhankov, A., Plöchl, L., and Slattery, K.T., "Assessment of tungsten for use in the ITER plasma facing components¹". *Journal of Nuclear Materials*, 1998. **258–263, Part 1**(0): p. 308-312.
- [31]. Ran, G., Wu, S., Liu, X., Wu, J., Li, N., Zu, X., and Wang, L., "The effect of crystal orientation on the behavior of a polycrystalline tungsten surface under focused Ga+

- ion bombardment". *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, 2012. **289**(0): p. 39-42.
- [32]. Was, G.S., "Fundamentals of radiation materials science: metals and alloys". 2007: Springer Science & Business Media.
- [33]. Tucker, R.P., Wechsler, M.S., and Ohr, S.M., "Dislocation Channeling in Neutron-Irradiated Niobium". *Journal of Applied Physics*, 1969. **40**(1): p. 400-408.
- [34]. Mastel, B., Kissinger, H.E., Laidler, J.J., and Bierlein, T.K., "Dislocation Channeling in Neutron-Irradiated Molybdenum". *Journal of Applied Physics*, 1963. **34**(12): p. 3637-3638.
- [35]. Gray, B.S., Brocklehurst, J.E., and McFarlane, A.A., "The irradiation induced plasticity in graphite under constant stress". *Carbon*, 1967. **5**(2): p. 173-180.
- [36]. Dodge, H.L., "Young's Modulus of Drawn Tungsten and its Variation with Change of Temperature, Including a Determination of the Coefficient of Expansion". *Physical Review*, 1918. **11**(4): p. 311-315.
- [37]. Farrell, K. and Byun, T.S., "Tensile properties of candidate SNS target container materials after proton and neutron irradiation in the LANSCE accelerator". *Journal of Nuclear Materials*, 2001. **296**(1-3): p. 129-138.
- [38]. Dai, Y., Maloy, S.A., Bauer, G.S., and Sommer, W.F., "Mechanical properties and microstructure in low-activation martensitic steels F82H and Optimax after 800-MeV proton irradiation". *Journal of Nuclear Materials*, 2000. **283-287**, **Part 1**(0): p. 513-517.
- [39]. Maloy, S.A., James, M.R., Willcutt, G., Sommer, W.F., Sokolov, M., Snead, L.L., Hamilton, M.L., and Garner, F., "The mechanical properties of 316L/304L stainless steels, Alloy 718 and Mod 9Cr-1Mo after irradiation in a spallation environment". *Journal of Nuclear Materials*, 2001. **296**(1-3): p. 119-128.

- 1
2
3
4
5 [40]. Toloczko, M.B., Hamilton, M.L., and Maloy, S.A., "High temperature tensile testing
6 of modified 9Cr–1Mo after irradiation with high energy protons". *Journal of Nuclear*
7 *Materials*, 2003. **318**(0): p. 200-206.
8
9
10
11 [41]. Zerilli, F.J. and Armstrong, R.W., "Dislocation-mechanics-based constitutive relations
12 for material dynamics calculations". *Journal of Applied Physics*, 1987. **61**(5): p. 1816-
13 1825.
14
15
16
17 [42]. Lennon, A.M. and Ramesh, K.T., "The thermoviscoplastic response of polycrystalline
18 tungsten in compression". *Materials Science and Engineering: A*, 2000. **276**(1–2): p.
19 9-21.
20
21
22
23 [43]. Zerilli, F.J. and Armstrong, R.W., "Description of tantalum deformation behavior by
24 dislocation mechanics based constitutive relations". *Journal of Applied Physics*, 1990.
25 **68**(4): p. 1580-1591.
26
27
28
29 [44]. Chen, S. and Gray, G., "Constitutive behavior of tantalum and tantalum-tungsten
30 alloys". *Metallurgical and Materials Transactions A*, 1996. **27**(10): p. 2994-3006.
31
32
33
34 [45]. Škoro, G.P., Bennett, J.R.J., Edgecock, T.R., and Booth, C.N., "Yield strength of
35 molybdenum, tantalum and tungsten at high strain rates and very high temperatures".
36 *Journal of Nuclear Materials*, 2012. **426**(1–3): p. 45-51.
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60
61
62
63
64
65

FIGURE CAPTIONS

Figure 1 Comparison of experiment results and predictions from the used Anand's model with material parameters obtained from the present study of saturation stress for (a) unirradiated W and (b) irradiated W.

Figure 2 Finite element (FE) model and mesh summary of (a) Unirradiated W, (b) Irradiated W (stage1), (c) Irradiated W (stage2), and (d) Irradiated W (stage 3). These FE models are constructed based on images of W microstructure given in (Ran et al. 2012).

Figure 3 Finite element mesh convergence test: von-Mises stress at indicated location (Element A) as a function of mesh elements.

Figure 4 Unirradiated tungsten: (a) Stress distribution and (b) Von-Mises stress-strain relation at the element A (shown earlier in Fig. 4).

Figure 5 Irradiated (stage 1) tungsten: (a) Stress distribution and (b) Von-Mises stress-strain relation at the element A (shown earlier in Fig. 4).

Figure 6 Irradiated (stage 2) tungsten: (a) Stress distribution and (b) Von-Mises stress-strain relation at the element A (shown earlier in Fig. 4).

Figure 7 Irradiated (stage 3) tungsten: (a) Stress distribution and (b) Von-Mises stress-strain relation at the element A (shown earlier in Fig. 4).

Figure 8 Comparison of experiments (Maloy et al. 2005) and the present study of yield strength of tungsten as a function of irradiation dose.

Figure 9 Yield strength of unirradiated and irradiated tungsten as a function of temperature.

LIST OF TABLES

Table 1. Summary of stress and plastic strain for unirradiated and irradiated W grains (Maloy et al. 2005)

Table 2. Young's modulus and Poisson's ratio for unirradiated and irradiated W grains (Smid et al. 1998, Dodge 1918)

Table 3. Obtained material parameters of unirradiated and irradiated W for the Anand model used in this work

Table 4. Initial value of internal variable (S_0) for unirradiated and irradiated W used in Eq. (10)

Table 5. Hardening parameter (h_0) for unirradiated and irradiated W used in Eq. (11)

Table 6. Young's modulus and Poisson's ratio for the W $\Sigma 31$ GB (Han and Tomar 2013).

Table 7. Summary of stress and plastic strain for the W $\Sigma 31$ GB (Han and Tomar 2013).

Table 8. Comparison between this work and previous result on Z&A model parameters for unirradiated tungsten. The parameter C_4 was determined using the curve fitting based on the simulation results.

Table 9. Material parameters used in the equation of the W microstructure yield strength (Eq. (16)).

Table 10. Comparison of the calculated values and predictions from the proposed relation of the W microstructure yield strength.

TABLE 1

Summary of stress and plastic strain for unirradiated and irradiated W grains (Maloy et al. 2005).

Unirradiated W			Irradiated W (stage 1)		
Temperature [K]	Stress [MPa]	Plastic Strain	Temperature [K]	Stress [MPa]	Plastic Strain
293	1300	0.00	293	1500	0.00
293	1450	0.048	293	1550	0.03
293	1600	0.08	293	1700	0.10
293	1700	0.14	293	1830	0.15
500*	800	0.00	433*	1550	0.00
500*	830	0.02	433*	1600	0.02
500*	980	0.075	433*	1800	0.075
748	470	0.00	433*	1900	0.125
748	500	0.02	748	900	0.00
748	650	0.075	748	929	0.02
748	700	0.10	748	1045	0.075
			748	1103	0.125
Irradiated W (stage 2)			Irradiated W (stage 3)		
Temperature [K]	Stress [MPa]	Plastic Strain	Temperature [K]	Stress [MPa]	Plastic Strain
298	1900	0.00	298	2100	0.00
298	1951	0.04	298	2130.44	0.05
298	2105	0.10	298	2206.52	0.10
298	2362	0.17	298	2252.17	0.175
433*	1850	0.00	495*	1380	0.00
433*	1900	0.04	495*	1400	0.05
433*	2050	0.10	495*	1450	0.10
433*	2300	0.17	495*	1480	0.175
748	1200	0.00	748	1300	0.00
748	1232	0.04	748	1319	0.05
748	1330	0.10	748	1366	0.10
748	1492	0.17	748	1394	0.175

* Determined through interpolation

TABLE 2

Young's modulus and Poisson's ratio for unirradiated and irradiated W grains (Smid et al. 1998, Dodge 1918).

Temperature [°C]	Young's Modulus [GPa]	Poisson's Ratio
20	355	0.28
200	350	
400	343	
600	337	
800	330	
1000	324	

TABLE 3

Obtained material parameters of unirradiated and irradiated W grain from the Anand model used in this work

Parameter	Unirradiated W	Irradiated W
Q/R (K)	190415.20	190583.58
A (1/sec)	1.0623×10^8	1.9058×10^8
ξ (dimensionless)	4	11
m (dimensionless)	0.00782	0.02606
$\hat{s}$ (MPa)	621.08	1430.55
n (dimensionless)	1.74567×10^{-4}	$- 2.7373 \times 10^{-4}$
a (dimensionless)	1.45	1.3

TABLE 4

Initial value of internal variable (S_0) for unirradiated and irradiated W grain used in Eq. (10)

Parameter	Unirradiated W	Irradiated W
S_1 (MPa)	23.018	-0.2124
S_2 (MPa/K)	1.2899	2.3581
S_3 (MPa/K ²)	- 2.6875 x 10 ⁻⁴	0.0

TABLE 5
Hardening parameter (h_0) for unirradiated and irradiated W grain used in Eq. (11)

Parameter	Unirradiated W	Irradiated W
A_1 (MPa)	838.05	- 606.15
A_2 (MPa/K)	49.737	1559.3
A_3 (MPa/K ²)	- 0.01041	- 0.00107

TABLE 6

Young's modulus and Poisson's ratio for the W Σ 31 GB (Han and Tomar 2013).

Temperature [K]	Young's Modulus [GPa]	Poisson's ratio
300	81	0.28
900	74	0.28

TABLE 7

Summary of stress and plastic strain for the W Σ 31 GB (Han and Tomar 2013).

Temperature [K]	Stress [GPa]	Plastic Strain
300	22	0.00
300	20	0.07
300	15	0.15
300	13	0.24
900	21	0.00
900	20	0.08
900	16	0.15
900	13	0.24

TABLE 8

Comparison between this work and previous result on Z&A model parameters for unirradiated W. The parameter C_4 was determined using the curve fitting based on the simulation results.

Parameter	(Lennon and Ramesh 2000)	The present study
C_1 (MPa)	2749	2749
C_2 (K ⁻¹)	2.25×10^{-3}	2.25×10^{-3}
C_3 (K ⁻¹)	9.05×10^{-5}	9.05×10^{-5}
C_4 (MPa)	49.91	-208.09
C_5 (MPa)	194.5	194.5
n	0.0505	0.0505

TABLE 9

Material parameters used in the equation of W microstructure yield strength (Eq. (16)).

Parameter	The present study
C_1 (MPa)	2749
C_2 (K ⁻¹)	2.25×10^{-3}
C_3 (K ⁻¹)	9.05×10^{-5}
C_4 (MPa)	-208.09
C_5 (MPa)	194.5
n	0.0505
A (MPa)	774.16
B	0.1285
p	0.5347

TABLE 10

Comparison of the calculated values and predictions from the proposed relation of the W microstructure yield strength.

Temperautre [K]	Irradiation dose [dpa]	Simulation [MPa]	The proposed relation [MPa]
350	0.0	1140	1179
	4.6	1500	1683
	14.9	1890	1890
	22.5	1890	1930
450	0.0	900	927
	4.6	1520	1430
	14.9	1800	1638
	22.5	1560	1677
550	0.0	720	726
	4.6	1320	1230
	14.9	1590	1437
	22.5	1380	1477
650	0.0	600	566
	4.6	1110	1070
	14.9	1410	1276
	22.5	1320	1316
750	0.0	480	438
	4.6	900	942
	14.9	1200	1149
	22.5	1290	1189

LIST OF FIGURES

Figure 1 Comparison of experiment results and predictions from the used Anand's model with material parameters obtained from the present study of saturation stress for **(a)** unirradiated W and **(b)** irradiated W.

Figure 2 Finite element (FE) model and mesh summary of **(a)** Unirradiated W, **(b)** Irradiated W (stage1), **(c)** Irradiated W (stage2), and **(d)** Irradiated W (stage 3). These FE models are constructed based on images of W microstructure given in (Ran et al. 2012).

Figure 3 Finite element mesh convergence test: von-Mises stress at indicated location (Element A) as a function of mesh elements.

Figure 4 Unirradiated tungsten: **(a)** Stress distribution and **(b)** Von-Mises stress-strain relation at the element A (shown earlier in Fig. 4).

Figure 5 Irradiated (stage 1) tungsten: **(a)** Stress distribution and **(b)** Von-Mises stress-strain relation at the element A (shown earlier in Fig. 4).

Figure 6 Irradiated (stage 2) tungsten: **(a)** Stress distribution and **(b)** Von-Mises stress-strain relation at the element A (shown earlier in Fig. 4).

Figure 7 Irradiated (stage 3) tungsten: **(a)** Stress distribution and **(b)** Von-Mises stress-strain relation at the element A (shown earlier in Fig. 4).

Figure 8 Comparison of experiments (Maloy et al. 2005) and the present study of yield strength of tungsten as a function of irradiation dose.

Figure 9 Yield strength of unirradiated and irradiated tungsten as a function of temperature.

Figure 1 Comparison of experiment results (Steichen, 1976) and predictions from the used Anand's model with material parameters obtained from the present study of saturation stress for (a) unirradiated W and (b) irradiated W ($0.4 - 0.9 \times 10^{22} \text{ n/cm}^2$).

Figure 2 Finite element (FE) model and mesh summary of **(a)** Unirradiated W, **(b)** Irradiated W (stage1), **(c)** Irradiated W (stage2), and **(d)** Irradiated W (stage 3). These FE models are constructed based on images of W microstructure given in (Ran et al. 2012).

Figure 3 Finite element mesh convergence test: von-Mises stress at indicated location (Element A) as a function of mesh elements.

Figure 4 Unirradiated tungsten: (a) Stress distribution and (b) Von-Mises stress-strain relation at the element A (shown earlier in Fig. 4).

Figure 5 Irradiated (stage 1) tungsten: (a) Stress distribution and (b) Von-Mises stress-strain relation at the element A (shown earlier in Fig. 4).

Figure 6 Irradiated (stage 2) tungsten: (a) Stress distribution and (b) Von-Mises stress-strain relation at the element A (shown earlier in Fig. 4).

Figure 7 Irradiated (stage 3) tungsten: (a) Stress distribution and (b) Von-Mises stress-strain relation at the element A (shown earlier in Fig. 7.4).

Figure 8 Comparison of experiments (Maloy et al. 2005) and the present study of yield strength of tungsten as a function of irradiation dose.

Figure 9 Yield strength of unirradiated and irradiated tungsten as a function of temperature.