Journal of Nuclear Materials 485 (2017) 231–242

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

A dislocation-based crystal viscoplasticity model with application to micro-engineered plasma-facing materials

David Rivera, Yue Huang, Giacomo Po, Nasr M. Ghoniem*

Department of Mechanical & Aerospace Engineering, University of California at Los Angeles (UCLA), 420 Westwood Plaza, Los Angeles, CA 90095-1597, USA

ARTICLE INFO

Article history:
Received 25 September 2016
Received in revised form
20 November 2016
Accepted 28 December 2016
Available online 30 December 2016

Keywords:
Tungsten
Thermomechanics
Plasma transients
Surface architecture
Residual stress

ABSTRACT

Materials developed with special surface architecture are shown here to be more resilient to the transient thermomechanical environments imposed by intermittent exposures to high heat flux thermal loading typical of long-pulse plasma transients. In an accompanying article, we present experimental results that show the relaxation of residual thermal stresses in micro-engineered W surfaces. A dislocation-based model is extended here within the framework of large deformation crystal plasticity. The model is applied to the deformation of single crystals, polycrystals, and micro-engineered surfaces composed of a uniform density of micro-pillars. The model is utilized to design tapered surface micro-pillar architecture, composed of a Re core and W coatings. Residual stresses generated by cyclic thermomechanical loading of these architectures show that the surface can be in a compressive stress state, following a short shakedown plasma exposure, thus mitigating surface fracture.

1. Introduction

Plasma-facing materials (PFM) are required for a great number of technological applications, encompassing space electric propulsion devices, micro-electronics fabrication, fusion energy conversion, and pulsed power devices, just to name a few. Continued development of space Electric Propulsion (EP), fusion energy, and Pulsed Power (PP) systems relies on fundamental advances in our understanding of material performance and survival in extraordinarily severe environments. The demand of higher performance materials is even greater in future technologies that will require materials to operate in substantially more aggressive environments. In such applications, PFM encounter unprecedented severe thermomechanical environments, as plasma ions and electrons slam onto the surface. Many physical degradation phenomena ensue, including material loss by ablation, blistering, sputtering and evaporation, as well as genuine thermoemchanical damage in the form of extensive plastic deformation and complex surface cracking.

To understand thermomechanical damage induced by intermittent high heat flux, one has to consider the main driver of damage accumulation, namely plastic deformation of some material regions that are constrained from expansion by cooler regions, or by external boundary conditions. Transient high heat flux induces a temperature gradient across PFM, which if constrained from bending or lateral expansion, can result in thermal stresses that exceed the yield point of the material. Considerations of cooling would require that a mechanical force, generated by the fluid pressure on the cold side, would also act on the PFM simultaneously with the thermal stress. While the mechanical force is generally constant, the thermal stress will fluctuate with each cycle, as the plasma heat source is turned on and off. Several interacting phenomena and manifestations of thermomechanical damage may take place under these specialized loading conditions; encompassing purely elastic response, shakedown behavior, reverse plasticity with ratcheting, viscoplastic deformation, and surface fracture. Considerations of the possibility of these outcomes, and finding solutions to mitigate the accumulation of

---

* Corresponding author.
E-mail address: ghoniem@ucla.edu (N.M. Ghoniem).

http://dx.doi.org/10.1016/j.jnucmat.2016.12.034
0022-3115/

thermomechanical damage through materials design are desirable pursuits in the development of resilient PFM for many demanding applications. We review briefly here related research on these phenomena as motivating background for the present work. We will first discuss classical approaches of elasto-plasticity employed for the solution of this problem. Since these approaches will be shown to have serious limitations and approximations, we will then review more fundamental modeling strategies that are based on including microstructure information. A discussion of experimental testing methods will be given, followed by engineering design approaches that are used to mitigate thermomechanical damage effects.

Classical methods of elasto-plasticity were developed to describe cyclic plasticity, often based on assumptions of the constitutive behavior of the material in a thermomechanical environment. Structural models for the analysis of residual thermal stresses in structures falls into two main simplifications: (1) connected bars that expand/contract at different rates upon uniform heating; and (2) beam/membranes that are prevented from bending and are subject to a temperature gradient. For example, Parkes [1] studied the problem of thermal ratchetting in an aircraft wing, and assumed it to be a two-bar structure in which the temperature of one bar is cycled while the temperature of the other bar is kept constant. Jiang and Leckie [2] presented a method for direct determination of the steady solutions in shakedown analysis of the two-bar problem. On the other hand, Bree [3] analyzed the elastic-plastic behavior of a thin cylindrical tube subjected to constant internal pressure and cyclic temperature drop across the tube thickness. He used a simple one-dimensional model, assumed a constant temperature gradient across the tube thickness and an elastic-perfectly plastic constitutive model. Many other researchers expanded on the basic Bree model of cyclic plasticity by considering kinematic hardening [4], creep effects [5], and shakedown loads with hardening [6]. These considerations are based on the idea of neglecting the axial stress in internally pressurized thin tubes, and applying equilibrium conditions on hoop stresses. When one introduces an elastic-perfectly plastic material model, four main regimes of behavior arise during cyclic thermal loading. At low mechanical (pressure) and thermal stress ranges, elastic behavior is expected (E-regime). As the temperature gradient increases with little increase in the mechanical stress, the cross-section becomes fully plastic (P-regime). At high values of mechanical and thermal stresses, thin structures enter into a ”ratcheting, or R-regime.” At moderate values of both thermal and mechanical stresses, the structure undergoes shake-down for a few cycles and settles with elastic behavior thereafter. The details of these four possibilities have been worked out by Bree [3], and have been incorporated into high temperature design codes [7–9].

Despite the success of classical elasto-plasticity methods in design applications (e.g. the adoption of the Bree diagram by the ASME design code for high temperature components [7–9]), they are limited in describing severe plasma transient effects on PFM. For example, Bree's original analysis was based on an elastic perfectly plastic, one-dimensional stress model of residual stresses, where material properties are assumed not to change from cycle-to-cycle. However, high temperature deformation entails a variety of physical phenomena such as dislocation climb, recovery, recrystallization, and subgrain growth, in addition to traditional dislocation glide mechanisms accompanying plastic deformation. All of these mechanisms become active to varying degrees by the presence of an elevated temperature (typically $> 0.4\,T_m$), and lead to gradual changes in the constitutive behavior of the material as severe thermal cycles are applied to it. The lack of any physical input into the thermomechanics of high heat flux components casts doubt on the predictive qualities of classical model. For these reasons, physically-based approaches, where dislocations are modeled as the basic carriers of plastic deformation, can lead to greater insight into the nature of thermomechanical damage accumulation.

The primary aim of the visco-plastic formulation presented here is to describe the thermomechanical response of PFM on a physical basis, where the microstructure (dislocations and grains) is represented. Among the earliest of microstructure-based plasticity models is a formulation by Kocks and Mecking (KM - model) [10–12]. The KM - model assumes that the strain rate, temperature, and internal parameters such as dislocation density (ρ), all play a role in determining the flow stress. This, in turn, follows the well-known Taylor hardening relation, namely that $\sigma = s(\dot{\varepsilon}, T)\widehat{\alpha}\mu b\sqrt{\rho}$, where $s(\dot{\varepsilon}, T)$ is a rate sensitive function, $\widehat{\alpha}$ is a constant on the order of unity, and μ is the shear modulus. This flow stress depends only on the resistance to deformation offered by the presence of dislocations. Since hardening or softening can occur as a result of dislocation-dislocation interactions, both the hardening and recovery rates have to be modeled. The Taylor hardening relationship in the KM model is written as: $\sigma d\sigma/d\varepsilon = (\alpha\mu b)^2/2 \times d\rho/d\varepsilon$, where the dislocation density is assumed to be a function of the strain via a rate equation that balances dislocation production with further straining and its rate of recovery, as: $d\rho/d\varepsilon = (\Lambda b)^{-1} - L_r N_r \nu_r/\dot{\varepsilon}$. The first term in the equation describes the rate of dislocation storage; while the second is the dynamic recovery rate. Λ is the mean free path a dislocation travels before it is annihilated or ceases to contribute to the plastic flow of the material, it is assumed to be proportional to the dislocation spacing $1/\sqrt{\rho}$, L_r is the length of dislocation segments, N_r is the dislocation density, and ν_r is the rate at which the dislocations are rearranged. The glide kinetics of the model can be described with an Arrhenius equation of the form: $\dot{\varepsilon} = \dot{\varepsilon}_o \exp - \frac{\Delta G(s_A)}{kT}$. The activation energy for dislocation glide $\Delta G(s_A)$ is dependent on stress and is given by: $s \equiv \frac{\sigma}{\widehat{\sigma}} = \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_o}\right)^{1/m}$, where $\widehat{\sigma}$ is the flow stress at 0 K, and m is the strain rate sensitivity.

Following similar lines to the KM approach, dislocation density based plasticity models have been advanced. Estrin et al. [13]. developed a model, which takes into account the cellular nature of the dislocation microstructure, and adequately described stages III, IV, and V of the stress-strain curve. Prinz and Argon similarly developed a framework by which stages III and IV of the stress-strain curve were accurately predicted [14]. Temporal dynamical behavior and spatial patterning have been analyzed with dislocation density models. Kubin and Estrin described the critical conditions for the Portevin-Le Chatelier effect [15], while the collective dynamical behavior of dislocations was investigated by Ananthakrishna [16], and by Kubin, Fressengeas, and Ananthakrishna [17]. Spatial patterning of dislocations in ordered structures, such as dislocation cells and Persistent Slip Bands (PSB) has been modeled with dislocation density equations by Walgraef and Aifantis [18–20], and extensively by Aifantis [21]. On the other hand, Kamada and Zikry developed a 3-D dislocation-based model, and applied the model to the deformation of intermetallics [22], and the effects of grain boundaries on large-strain deformation was also studied [23]. Several applications of the model were extended to other material systems [24,25]. Arsenlis and Parks developed a dislocation-density based model to study the crystallographic aspects of geometrically-necessary and statistically-stored dislocation densities [26], and the evolution of crystallographic dislocation density in crystal plasticity [27].

It is interesting to note that despite the wide variety of dislocation-based models of plasticity [28], there have been relatively few formulations which explicitly incorporate high