SIMULATION OF DYNAMIC POLYCRYSTALLINE THERMOELASTOVISCOPLASTICITY AND FRACTURE

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Summary Presented is a framework for modeling the dynamic response of multi-phase polycrystalline microstructures, accounting for finite deformations, rate dependence of flow stress, thermal softening, thermal expansion, heat conduction, and thermoelastic coupling. Fracture is simulated via the cohesive zone approach. Aspects associated with constitutive modeling of anisotropic damage in the homogenized material system are discussed in light of the results.

INTRODUCTION

Tungsten Heavy Alloys (WHAs) are attractive candidates for use as kinetic energy penetrators because of their relatively large mass density, high melting point, and high strength at elevated rates of loading. The material studied here consists of relatively stiff and brittle pure tungsten grains (BCC), most often nearly equi-axed in shape, embedded in a relatively compliant and ductile matrix (FCC) consisting of nickel, iron, and tungsten. Experimental [1] and numerical [2] methods have demonstrated a clear correlation between lattice orientation of W single crystals and the performance of such crystals as kinetic energy penetrators. The potential exists for development of more descriptive constitutive models accounting for local crystallographic orientation effects, models which would simultaneously engender more accuracy to ballistic simulations and support design of microstructures tailored for enhanced thermomechanical properties. The present work employs single crystalline plasticity models for the constituent phases of the WHA. Models for both materials are embedded within a general thermodynamic framework applicable for describing any thermoelastic-viscoplastically-deforming single crystal. Previous investigations [3, 4] reveal a variety of failure modes exhibited by WHAs strained at high rates, including brittle fracture at W-W grain boundaries, transgranular cleavage of W grains, matrix-grain decohesion, ductile matrix rupture, and adiabatic shear banding. Recent high rate experiments of Weerasooriya [4] indicate that tensile failure of WHA specimens often initiates via local fracture at W-W (i.e., grain-grain) interfaces and less often at interfaces between W grains and the matrix phase. In our framework, we model interface fracture by invoking the cohesive zone approach [5].

CONSTITUTIVE THEORY

A multiplicative decomposition of the local deformation gradient $\mathbf{f}$ is assumed as follows:

$$\mathbf{f} = \partial\mathbf{x}/\partial\mathbf{X} = \mathbf{f}^{\mathbf{e}}\mathbf{f}^{\mathbf{\theta}}\mathbf{f}^{\mathbf{p}}, \tag{1}$$

with spatial coordinates $\mathbf{x} = \mathbf{x}(\mathbf{X},t)$, $\mathbf{f}^{\mathbf{e}}$ the elastic deformation, $\mathbf{f}^{\mathbf{\theta}}$ the stress-free thermal deformation, and $\mathbf{f}^{\mathbf{p}}$ the plastic deformation due to dislocation glide. Time rates of thermal and plastic deformation gradients are described by

$$\dot{\mathbf{f}}^{\mathbf{\theta}}\mathbf{f}^{\mathbf{\theta}-1} = \alpha\dot{\theta}\mathbf{1}, \qquad \dot{\mathbf{f}}^{\mathbf{p}}\mathbf{f}^{\mathbf{p}-1} = \sum_{\alpha=1}^{n}\dot{\gamma}^{(\alpha)}\mathbf{s}_0^{(\alpha)}\otimes\mathbf{m}_0^{(\alpha)}, \tag{2}$$

where $\dot{\gamma}^{(\alpha)}$, $\mathbf{s}_0^{(\alpha)}$, and $\mathbf{m}_0^{(\alpha)}$ are slip system shearing rates, referential slip directors, and referential slip plane normals, respectively. Also, θ is the absolute temperature, and α is the coefficient of (isotropic) thermal expansion. The Helmholtz free energy per unit mass, ψ, has the following functional form:

$$\tilde{\rho}\psi = \tilde{\rho}\psi\left(\mathbf{e}^{\mathbf{e}},\theta,\xi\right) = \underbrace{\frac{1}{2}\mathbf{e}^{\mathbf{e}}:\mathbf{c}(\theta,\xi):\mathbf{e}^{\mathbf{e}}}_{hyperelasticity} + \underbrace{\frac{1}{2}\kappa\mu(\theta,\xi)\xi^2}_{lattice\,defects} + \underbrace{y(\theta)}_{\substack{heat\\energy}}, \tag{3}$$

with $\tilde{\rho}$ the mass density in the relaxed intermediate configuration, $2\mathbf{e}^{\mathbf{e}} \equiv \mathbf{f}^{\mathbf{e}T}\mathbf{f}^{\mathbf{e}} - \mathbf{1}$ an elastic strain, $\mathbf{c}$ the elastic modulus, $\xi \equiv b\sqrt{\rho_T}$ a dimensionless internal variable associated with the total dislocation density ρ_T and burgers vector b, κ a material parameter, and μ an elastic shear modulus. The localized spatial energy balance becomes

$$\underbrace{\rho c_p\dot{\theta}}_{\substack{temperature\\change}} = \underbrace{\sum_{\alpha=1}^{n}\tau^{(\alpha)}\dot{\gamma}^{(\alpha)}}_{\substack{plastic\\dissipation}} - \underbrace{\rho\left((\partial_\xi\psi) - \theta(\partial_{\theta\xi}\psi)\right)\dot{\xi}}_{\substack{energy\,of\\lattice\,defects}} + \underbrace{\rho\theta\partial_{\theta\mathbf{e}^{\mathbf{e}}}\psi:\dot{\mathbf{e}}^{\mathbf{e}}}_{thermoelastic\,coupling} + \underbrace{div(k\nabla_{\mathbf{x}}\theta)}_{\substack{heat\\conduction}}, \tag{4}$$

where ρ is the current mass density, c_p is the specific heat capacity, $\tau^{(\alpha)}$ is the resolved Cauchy stress on system α, and k is the thermal conductivity. Evolution of the plastic deformation is specified by a viscoplastic flow rule

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \left\{ \tilde{\tau}^{(\alpha)} \left(\theta_0 / \theta \right)^p / g_0^{(\alpha)} \right\}^m \mathrm{sgn} \left(\tilde{\tau}^{(\alpha)} \right), \tag{5}$$

where $\tilde{\tau}^{(\alpha)}$ is a resolved Kirchhoff stress, $g_0^{(\alpha)}$ a slip resistance under isothermal conditions, p a thermal softening exponent, m the strain rate sensitivity, and $\dot{\gamma}_0$ and θ_0 material parameters. The dislocation density ρ_T evolves in conjunction with changes in the average strength of all slip systems. Intergranular fracture events at interfaces between W grains and at grain-matrix interfaces are captured by cohesive models in which the interfacial load decreases linearly with separation distance (i.e., crack opening displacement) upon attainment of a critical stress level at the interface [5].

NUMERICAL SIMULATIONS AND RESULTS

The above constitutive model was implemented within the EPIC dynamic wave propagation finite element code [6]. Meshes of triangular elements were generated using the PPM2OOF software package [7], readily enabling meshing of digital images with refinement along material interfaces (i.e., mesh refinement along potential cohesive fracture surfaces). Figure 1 shows the deformed grid from a representative 2D calculation: a large crack has developed along the interface shared by three W crystals, and two smaller cracks have opened at the lateral boundaries. Results from parametric studies show the effects of initial crystallographic texture and relative failure strengths of the interface types upon the net flow stress and crack initiation and propagation within the volume element.
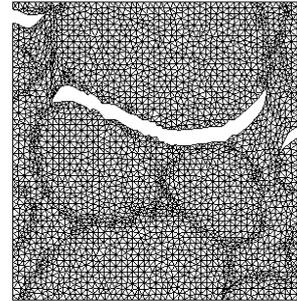

Figure 1. Deformed mesh.

MACROSCOPIC DAMAGE MODEL

An important objective of the present work is support of the construction of physically realistic macroscopic models of the kinematics, thermodynamics, and kinetics of fully anisotropic damage for subsequent implementation in design codes. Addressing the kinematics, the homogenized deformation gradient $\mathbf{F}$ for a damaged material element containing k internal surfaces can be decomposed as [8]

$$\mathbf{F} \equiv \frac{1}{V} \int_S \mathbf{x} \otimes \mathbf{n} \, dS = \frac{1}{V} \int_V \mathbf{f} \, dV + \frac{1}{V} \sum_k \int_{S^{(k)}} \mathbf{x} \otimes \mathbf{n} \, dS^{(k)} = \mathbf{F}^{\mathbf{m}} + \mathbf{F}^{\mathbf{d}}, \tag{6}$$

where S is the external surface of the volume element of referential volume V, with unit surface normal vector $\mathbf{n}$. In Eq. (6), $\mathbf{F}^{\mathbf{m}}$ is the deformation gradient contribution from the intact material, and $\mathbf{F}^{\mathbf{d}}$ is the contribution from internal surface discontinuities associated with damage (e.g., cracks, voids, and shear bands). For the tensile-type fracture modes observed in experiments [4] and our numerical calculations, we propose the following simplified evolution laws:

$$\mathbf{F}^{\mathbf{d}} = \Lambda \left(\mathbf{F}^{\mathbf{m}} - \mathbf{1} \right), \qquad \dot{\Lambda} = \dot{\Lambda} \left(\mathbf{T}, t \right), \qquad \mathbf{F}^{\mathbf{d}} \left(t = 0 \right) = \mathbf{0}, \tag{7}$$

with $\mathbf{T}$ the net first Piola-Kirchhoff stress for the volume element and Λ a stress state dependent history variable—nonzero upon attainment of a critical nucleation criterion—scaling the rate of deformation accommodation from damage. For a given imposed total deformation gradient $\mathbf{F}$, the greater the magnitude of $\mathbf{F}^{\mathbf{d}}$, the less strain remaining to be accommodated by the net elastic part of $\mathbf{F}^{\mathbf{m}}$, resulting in a reduction in magnitude of the net stress.

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