4.1 PRELIMINARY PROGRESS IN THE DEVELOPMENT OF DUCTILE-PHASE TOUGHENED TUNGSTEN FOR PLASMA-FACING MATERIALS: DUAL-PHASE FINITE ELEMENT DAMAGE MODELS

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OBJECTIVE

The objective of this study is to develop a finite element continuum damage model suitable for modeling deformation, cracking, and crack bridging for W-Cu, W-Ni-Fe, and other ductile phase toughened W-composites, or more generally, any multi-phase composite structure where two or more phases undergo cooperative deformation in a composite system.

SUMMARY

A promising approach to increasing fracture toughness and decreasing the DBTT of a W-alloy is by ductile-phase toughening (DPT) [1-3]. In this method, a ductile phase is included in a brittle matrix to prevent fracture propagation by crack bridging or crack deflection. Liquid-phase sintered W-Ni-Fe alloys and hot-pressed and sintered W-Cu composites are two examples of such materials that PNNL and UCSB are investigating. However, there is a need for improved mechanical property models of such composite systems in order to begin to optimize these structural materials with regard to strength and fracture toughness. This report describes such a model that is currently under development at PNNL.

PROGRESS AND STATUS

Background

Tungsten (W) and W-alloys are the solid materials of choice for plasma-facing components (PFCs) of future fusion reactors, such as the International Thermonuclear Experimental Reactor (ITER) and Demonstration Power Plant (DEMO), due to their high melting point, strength at high temperatures, high thermal conductivity, low coefficient of thermal expansion, and low sputtering yield [4-8]. However, W and most W-alloys exhibit low fracture toughness and a high ductile-brittle transition temperature (DBTT) that would render them as brittle materials during reactor operations [4, 6, 9]. The DBTT for unirradiated W-alloys typically ranges from 573K to 1273K (300 to 1000˚C) and in a reactor environment radiation hardening would further elevate this range [6, 10, 11]. W-alloys toughened by engineered reinforcement architectures, such as ductile-phase toughening (DPT), are strong candidates for PFCs. In DPT, a ductile phase is included in a brittle matrix to prevent fracture propagation. The principles of DPT are illustrated in Figure 1, which shows an actual and schematic illustration of ductile bridging ligaments stretching across an open crack in a brittle matrix material, such as W [12, 13].

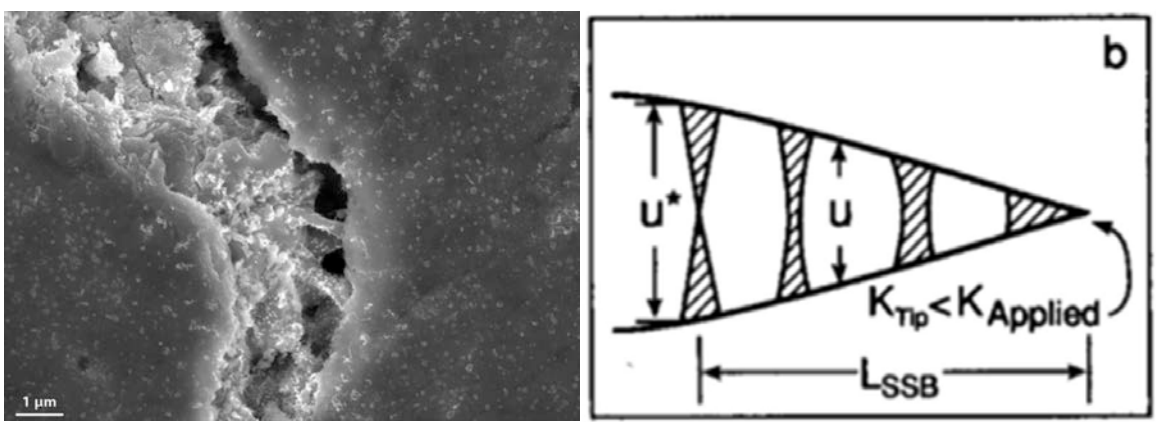


Figure 1. a) SEM image of W-Cu fracture where the ductile phase (Cu) is effectively bridging the crack. b) A steady-state bridging zone shown schematically in 2D [13].

Model Development

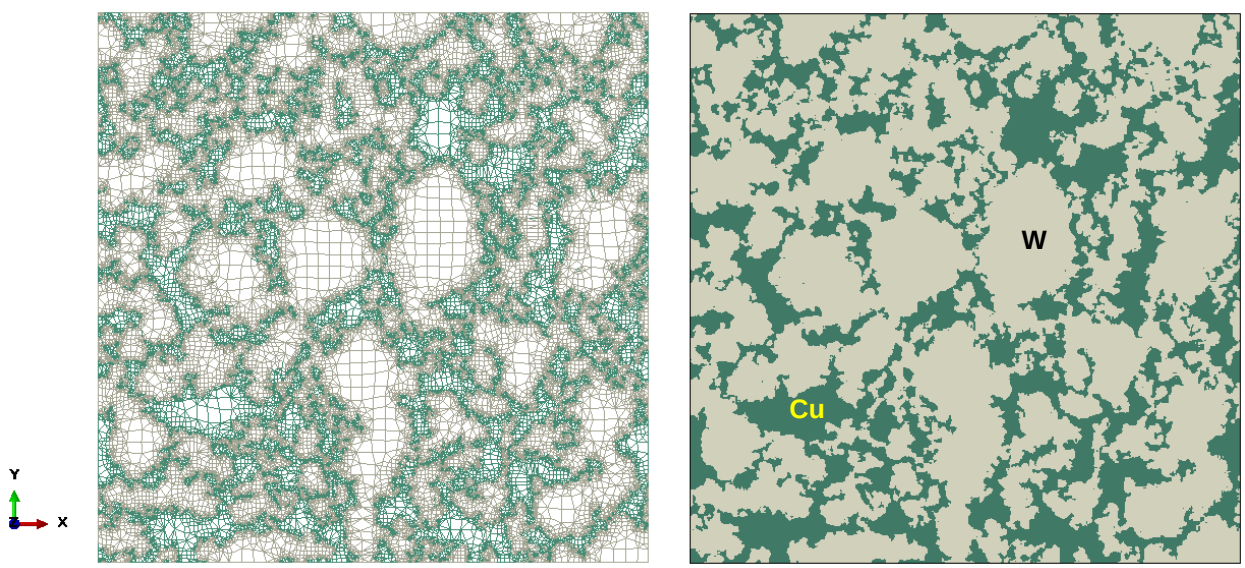
The specifics of the finite element continuum damage model (FE-CDM) developed at PNNL have been discussed previously [14, 15]. To understand how deformation proceeds, and how cracks initiate and

propagate in DPT W-composites, finite element analyses of W-composite specimens subjected to bending are being performed using the FE-CDM model for elastic and elastic-plastic materials. The CDM is implemented in the ABAQUS® finite element code via user defined subroutines. This CDM model derived from a model developed for long-fiber thermoplastic composites [16] is now being applied at the micron and submicron scale by creating dual-phase FE mesh regions in both 2D and 3D. The constitutive behavior of each phase in the modeling domain is described by the CDM to explore deformation, cracking, and crack bridging in these composite materials. Comparative analyses using an elastoplastic damage model available in ABAQUS are being performed to assess the predictions by this damage model . At this stage, the assessment and further development of the damage model are ongoing.

Summary of Approach

Damage in an elastic-plastic and damageable material can be described by a scalar variable, D, that can be related to the level of damage accumulation in the material [17]. Damage affects the material stiffness according to a stiffness reduction law. Using the concepts of thermodynamics of continuous media [17, 18], a thermodynamic potential is defined to derive the constitutive relations and the thermodynamic force associated with the damage variable. This CDM uses the density of the elastic deformation energy as the thermodynamic potential that provides a coupling between damage and elasticity-plasticity. A damage criterion dependent on a damage threshold function is defined and the damage evolution law is obtained. Damage evolves with deformation according to the damage evolution law until a critical (saturation) state at which $D=D_{\mathrm{cr}}$ $(0<D_{\mathrm{cr}}<1)$ and failure occurs. In this work, failure at damage saturation ($D=D_{\mathrm{cr}}$) leading to crack initiation and propagation is modeled by a vanishing finite element technique [19] that reduces the stiffness and stresses of the failed element to zero.

The FE mesh for these models is created from digital images of actual microstructures by using the public domain software OOF2[1] that creates multiple mesh domains with high-resolution elements at phase boundaries. The software allows the user to specify mechanical properties for each meshed region and outputs an input file for ABAQUS®. Figure 1 is an image of a W-Cu sample microstructure and its associated FE mesh.



(a) (b)

Figure 2. W-Cu composite with a FE mesh in (a) and the associated digital image in (b) with the phase regions identified. The mesh model contains two separate meshes each with its own set of mechanical properties.

[1] OOF2 was developed at the National Institute of Standards and Technology (NIST).

Figure 3 shows the stress-strain curves obtained from the literature for the two phases, W and Cu. These constitutive relations are applied to each phase as the model is deformed and failure occurs when the strains exceed the ultimate tensile strains. As a test of the model, the FE-CDM is deformed using uniaxial tension along the x-axis for the W-Cu meshed microstructure from Figure 2 as shown in Figure 4.

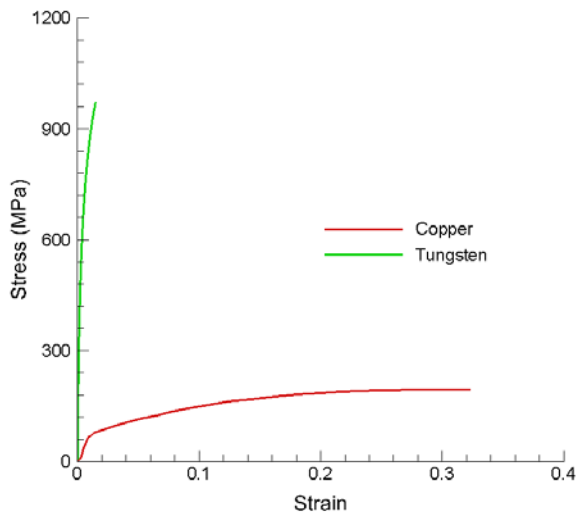


Figure 3. Constitutive relations for each of the two phases, W and Cu. The W phase is strong and brittle while the Cu phase is softer and much more ductile.

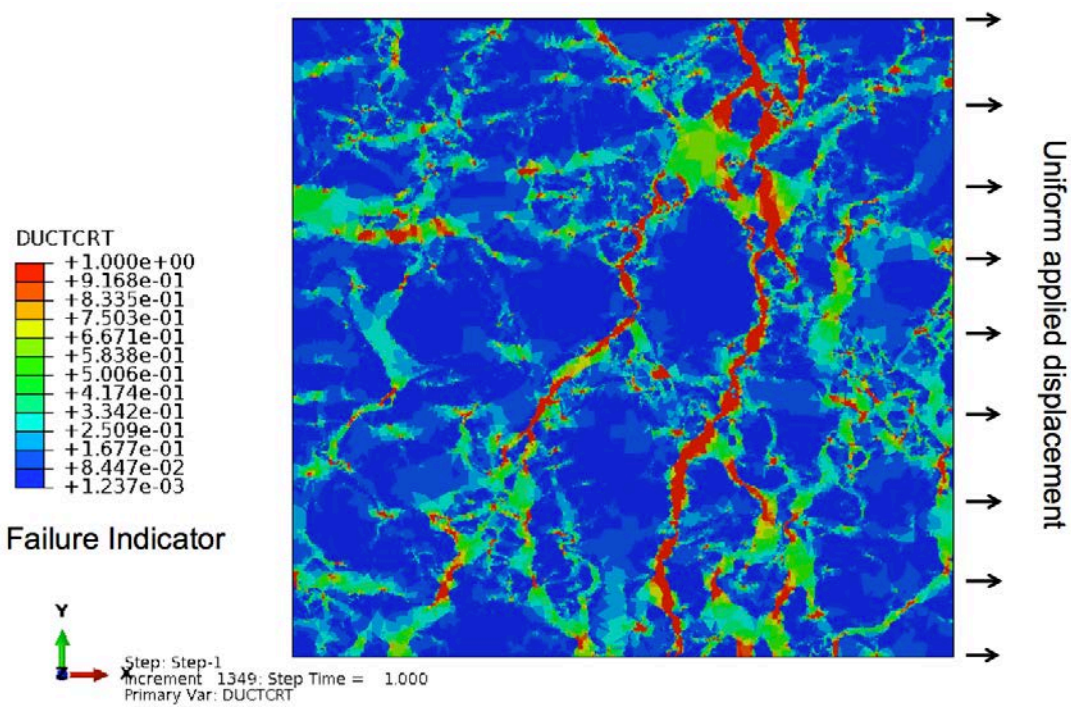


Figure 4. Damage model predictions of deformation in the W-Cu two-phase model. The red regions are failed regions that occur in the Cu phase. Highly stressed regions corresponding to increasing damage are shown in green-yellow-orange and are also found in the Cu phase. These damaged regions surrounded by failed regions would be considered to be ductile bridges in the W-Cu composite.

The FE-CDM approach is being extended to 3D as shown in Figure 5. The original 2D mesh model is extruded into 3D and stressed in uniaxial tension as before. The deformation map in terms of damage accumulation is shown in Figure 6. Note the differences in the amount and type of damage accumulation in the 3D map compared to the 2D map. The relevant overall stress-strain curves for the W-Cu composite is shown in Figure 7 comparing the 2D and 3D results. However, these results are preliminary as noted.

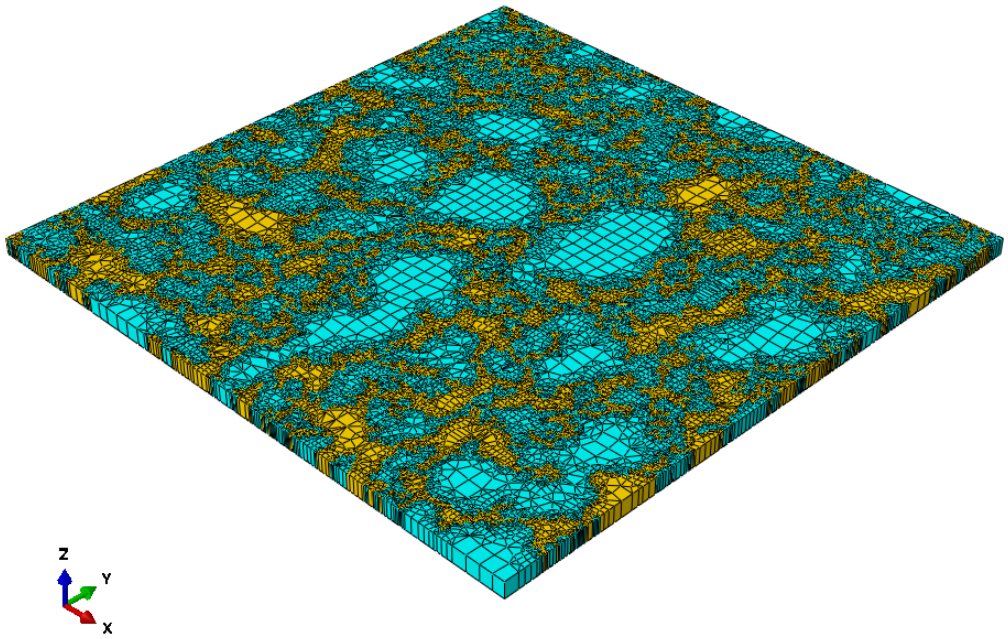
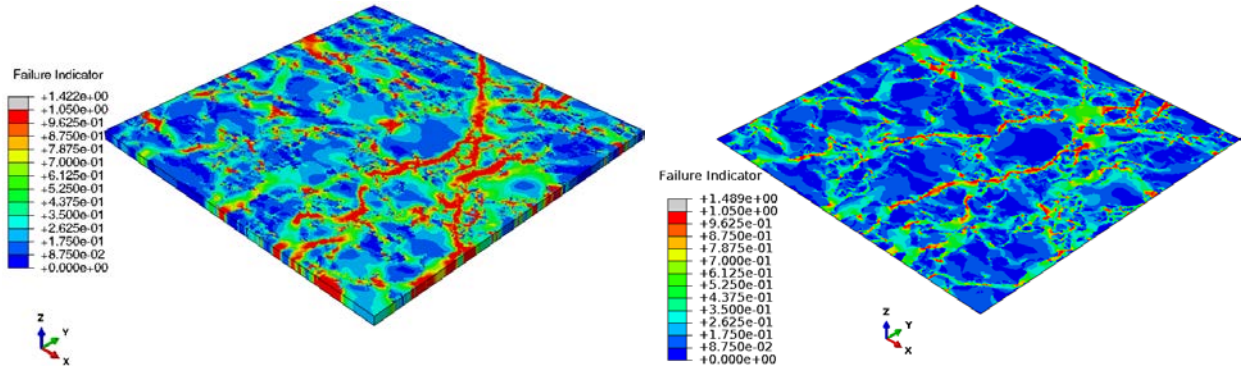


Figure 5. 3D FE mesh created by extruding the original 2D mesh. The blue regions are W and the gold regions are Cu.



(a) (b)

Figure 6. (a) 3D damage map under uniaxial tension in the x-direction and (b) is a 2D damage map under the same deformation. The damage accumulation is different in 3D compared to 2D.

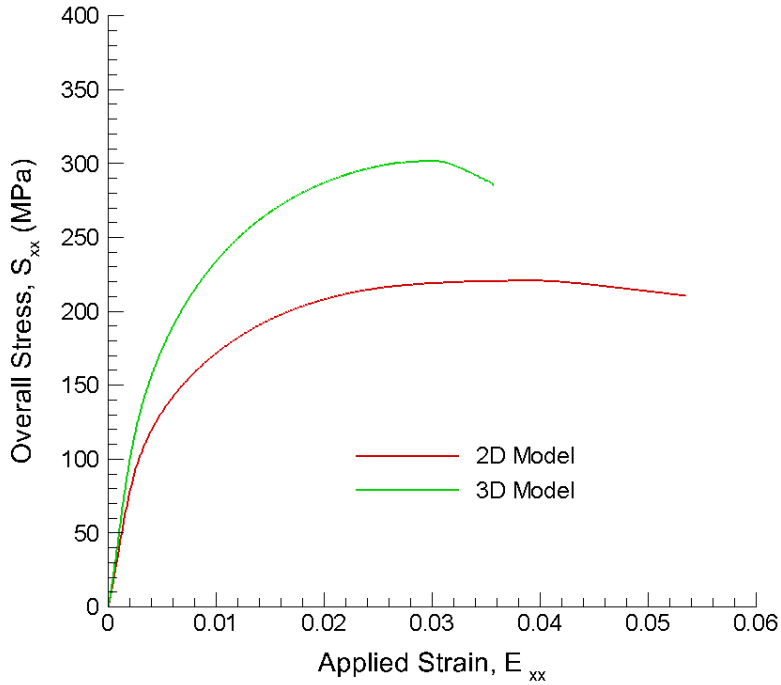


Figure 7. Composite stress-strain curves for the W-Cu composite strained in tension along the x-direction. The 3D model results predict a stronger but less ductile material as the loading in the 3D model appears to be shared more with the W phase.

Discussion

These preliminary results indicate the power of the FE-CDM approach in modeling the distributed damage observed in our experimental bend tests of this material. Our dynamic bridging model, while being able to describe the time and temperature dependence of the Cu flow stress with high accuracy was not able to describe the amount of load sharing observed in the bend sample that increased with increasing temperature [20]. Note that multiple cracking occurs naturally in the FE-CDM developed here but we did not yet perform simulations as a function of temperature. We have yet to show agreement with our experimental data except to note the similarities of the distributed cracking and damage in the W-Cu composite that was one of the most significant observations of cracking that we made in our experimental work with this material.

Future Work

Further model development will proceed along with generation of improved 3D mesh models of these W-Cu and W-Ni-Fe materials. We intend to create meshed models that correspond to actual 3D bend bar microstructures and to begin the process of model validation using SENB data.

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