4.2 PRELIMINARY PROGRESS IN THE DEVELOPMENT OF DUCTILE-PHASE TOUGHENED TUNGSTEN FOR PLASMA-FACING MATERIALS: DUAL-PHASE FINITE ELEMENT DAMAGE MODELS—C. H. Henager, Jr., B. N Nguyen, R. J. Kurtz (Pacific Northwest National Laboratory)

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 ductile-brittle transition temperature (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 [4-6]. However, W and most W-alloys exhibit low fracture toughness and a high DBTT that would render them as brittle materials during reactor operations [4, 6, 7]. 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, 8, 9]. 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 [10].

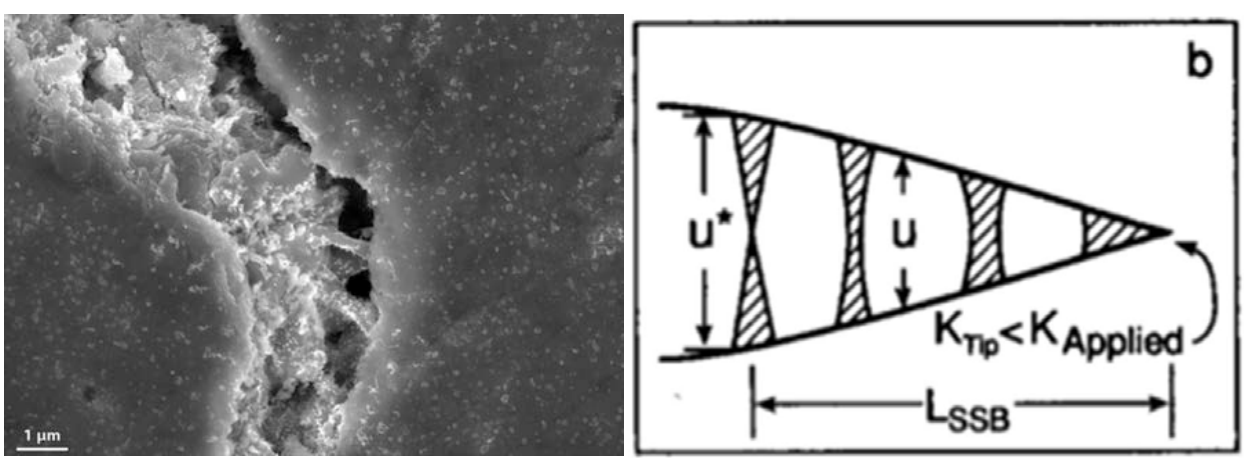


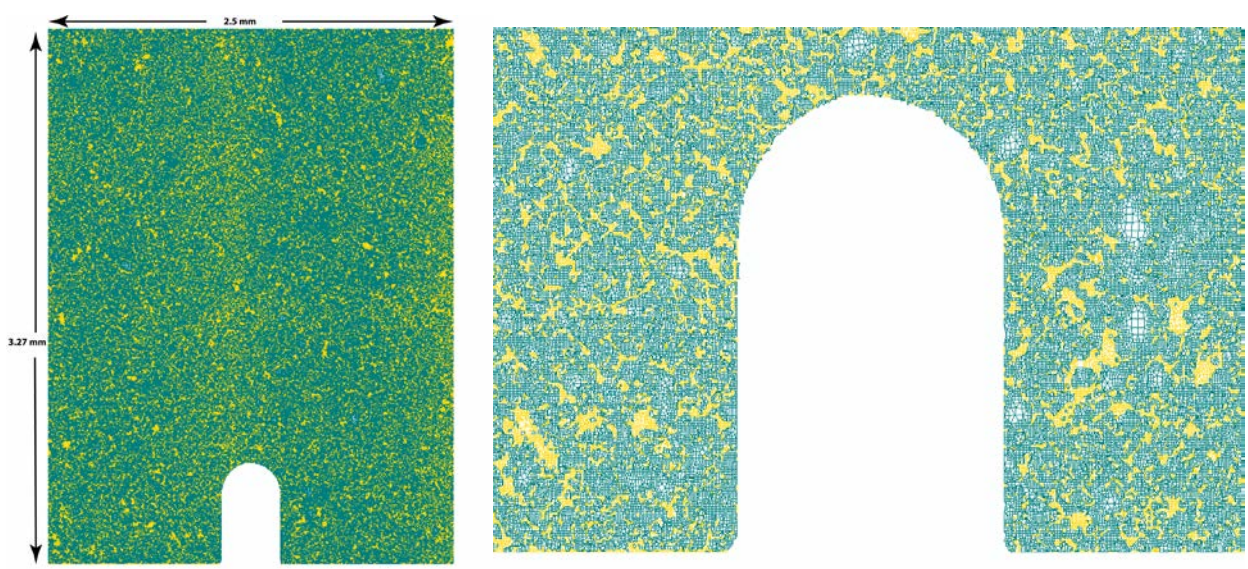
Figure 1. a) SEM image of W-Cu fracture where the ductile phase (Cu) is effectively bridging the crack. b) A steady-state bridging zone shown schematically in 2D [10].

Model Development

The specifics of the finite element continuum damage model (FE-CDM) developed at PNNL have been discussed previously [11, 12]. 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 [13] is now being applied at the micron and submicron scale by creating dual-phase FE mesh regions in both 2D and 3D for 3-point and 4-point bend bars for direct comparison to notched bend data. 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.

Summary of Approach

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 2 is an image of a W-Cu sample microstructure and its associated FE mesh for a notched bend bar.



(a) (b)

Figure 2. W-Cu composite with a FE mesh shown in (a) of the entire width and a portion of the length of a 3-point single-edge-notched beam (SENB) test bar that is 3.27 x 1.60 x 16.10 mm in size with a magnified region shown in (b) with the phase regions identified by color. Dark green is tungsten and light yellow is copper. The large mesh model in (a) contains two separate meshes each with its own set of mechanical properties and consists of more than 800K finite elements both triangular and quadrilateral types.

The approach is to create homogenized, meshed regions alongside the dual-phase meshed region shown in Figure 2a to create a fully meshed model of a bend bar that corresponds to the physical dimensions of our 3-point and 4-point bend samples. Thus, homogenized regions 3.27 x 6.8 mm will be created and added to the dual-phase meshed region shown in Figure 2a to achieve a full sized FE model

[1] OOF2 was developed at the National Institute of Standards and Technology (NIST). See http://www.ctcms.nist.gov/oof/oof2/.

of the 3-point SENB test bar. The dual-phase meshed region at the notch is required to capture the proper cracking patterns observed in the bending test of the W-composites.

The FE model will then be deformed in 3-point bending, for the case of the W-Cu composite shown in Figure 1, and the load-displacement response will be compared to the experimental data. The FE damage model predictions would also be compared to the actual cracking observed in the bend specimens. In this way, the use of the separate constitutive relations (see Figure 3) for tungsten and copper can be validated against experiment since there are uncertainties in assuming that bulk tungsten and bulk copper constitutive relations apply to these fine-scale W-Cu composites. Larger FE models will be similarly created for the 4-point SENB test bars used to study the newer W-Ni-Fe composites.

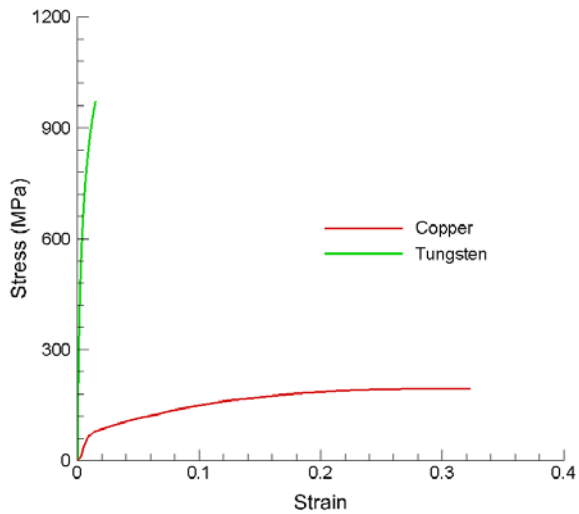


Figure 3. Constitutive relations initially assumed for each of the two phases, W and Cu, based on bulk behavior. The W phase is strong and brittle while the Cu phase is softer and much more ductile.

Discussion

This approach is anticipated to be an improvement over the dynamic bridging model previously developed and discussed to describe the amount of load sharing observed in the bend sample that increased with increasing temperature [14]. We had previously observed that multiple cracking occurs naturally in the FE-CDM model but we did not yet perform simulations as a function of temperature. We intend to show agreement with our experimental data with respect to load-displacement curves and to the distributed cracking and damage in the W-Cu composite that was one of the most significant observations made in our experimental work with this material.

Future Work

We will continue to create meshed models that correspond to actual 3D bend bar microstructures and to begin the process of model validation using SENB data.

References

[1] Deve, H.E., A.G. Evans, G.R. Odette, R. Mehrabian, M.L. Emiliani, and R.J. Hecht, Acta metallurgica et materialia, 1990. 38(8): p. 1491-502.
[2] Erdogan, F. and P.F. Joseph, J. Am. Ceram. Soc., 1989. 72(2): p. 262-270.
[3] Sigl, L.S., P.A. Mataga, B.J. Dalgleish, R.M. McMeeking, and A.G. Evans, Acta Metall., 1988. 36(4): p. 945-953.
[4] Rieth, M., J.L. Boutard, S.L. Dudarev, T. Ahlgren, S. Antusch, N. Baluc, M.F. Barthe, C.S. Becquart, L. Ciupinski, J.B. Correia, C. Domain, J. Fikar, E. Fortuna, C.C. Fu, E. Gaganidze, T.L. Galan, C.

Garcia-Rosales, B. Gludovatz, H. Greuner, K. Heinola, N. Holstein, N. Juslin, F. Koch, W. Krauss, K.J. Kurzydlowski, J. Linke, C. Linsmeier, N. Luzginova, H. Maier, M.S. Martinez, J.M. Missiaen, M. Muhammed, A. Munoz, M. Muzyk, K. Nordlund, D. Nguyen-Manh, P. Norajitra, J. Opschoor, G. Pintsuk, R. Pippan, G. Ritz, L. Romaner, D. Rupp, R. Schaublin, J. Schlosser, I. Uytdenhouwen, J.G. Van Der Laan, L. Veleva, L. Ventelon, S. Wahlberg, F. Willaime, S. Wurster, and M.A. Yar, J. Nucl. Mater., 2011. 417: p. 463-467.

[5] Pitts, R.A., A. Kukushkin, A. Loarte, A. Martin, M. Merola, C.E. Kessel, V. Komarov, and M. Shimada, Physica Scripta Volume T, 2009. 2009(T138): p. 014001 (10 pp.).

[6] Mertens, P., T. Hirai, M. Knaup, O. Neubauer, V. Philipps, J. Rapp, V. Riccardo, S. Sadakov, B. Schweer, A. Terra, I. Uytdenhouwen, and U. Samm, Fusion Eng. Des., 2009. 84(7-11): p. 1289-93.

[7] Mertens, P., V. Philipps, G. Pintsuk, V. Riccardo, U. Samm, V. Thompson, and I. Uytdenhouwen, Physica Scripta Volume T, 2009. 2009(T138): p. 014032 (5 pp.).

[8] Gludovatz, B., S. Wurster, A. Hoffmann, and R. Pippan, Int. J. Refract. Met. Hard Mater., 2010. 28(6): p. 674-8.

[9] Zinkle, S.J. and N.M. Ghoniem, Fusion Eng. Des., 2000. 51-52: p. 55-71.

[10] Odette, G.R., B.L. Chao, J.W. Sheckherd, and G.E. Lucas, Acta metallurgica et materialia, 1992. 40(9): p. 2381-9.

[11] Henager, C.H., B.N. Nguyen, R.J. Kurtz, T.J. Roosendaal, B.A. Borlaug, M. Ferraris, A. Ventrella, and Y. Katoh, J. Nucl. Mater., 2015. 466: p. 253-268.

[12] C. H. Henager, J., B.N. Nguyen, R.J. Kurtz, M. Ferraris, and Y. Katoh, in *Fusion Reactor Materials Program Semiannual Progress Reports*, Vol. 58, F. Wiffen, R. Godfrey, and B. Waddell, Editors. 2015, ORNL: Oak Ridge, TN. p. 108-118

[13] Nguyen, B.N. and V. Kunc, Int. J. Damage Mech., 2010. 19(6): p. 691-725.

[14] Cunningham, K.H., K. Fields, D. Gragg, F.W. Zok, J. C. H. Henager, R.J. Kurtz, and T. Roosendaal, in *DOE/ER-0313/54 - Volume 54, Semiannual Progress Report, June 30, 2013*, Vol. 54, F. Wiffen, R. Godfrey, and B. Waddell, Editors. 2013, US DOE: ORNL, TN. p. 95-107