3.2 LOW ACTIVATION JOINING OF SiC/SiC COMPOSITES FOR FUSION APPLICATIONS: MODELING MINIATURE TORSION TESTS WITH ELASTIC AND ELASTIC-PLASTIC MODELS – C.H. Henager, Jr., B.N. Nguyen, R.J. Kurtz, T. Roosendaal, and B. Borlaug; (Pacific Northwest National Laboratory[1], Richland, WA, USA); M. Ferraris, (Politecnico di Torino, Torino, Italy); A. Ventrella[2], and Y. Katoh, (Oak Ridge National Laboratory)

OBJECTIVE

Mechanics damage models that have been modified to better match torsion experiments involving elastic and elastic-plastic materials are presented to help formulate a path forward with joint testing and analysis for SiC materials in nuclear environments. This report extends the analysis from the last reporting cycle.

SUMMARY

The use of SiC and SiC-composites in fission or fusion environments requires joining methods for assembling systems. The international fusion community designed miniature torsion specimens for joint testing and irradiation in test reactors with limited irradiation volumes. These torsion specimens fail out-of-plane when joints are strong and when elastic moduli are within a certain range compared to SiC, which causes difficulties in determining shear strengths for joints or for comparing unirradiated and irradiated joints. A finite element damage model was developed that indicates fracture is likely to occur within the joined pieces to cause out-of-plane failures for miniature torsion specimens when a certain modulus and strength ratio between the joint material and the joined material exists. The model was extended to treat elastic-plastic joints such as SiC/epoxy and steel/epoxy joints tested as validation of the specimen design.

PROGRESS AND STATUS

Introduction

The international fusion materials community is currently irradiating several joint types and compositions in the HFIR reactor at ORNL [1]. PNNL is working with Politecnico di Torino and ORNL using miniature torsion specimens (hourglass samples) that have been specifically designed for pre- and post-irradiation joint shear strength testing [2]. Many of the joints fail out-of-plane, or in the base CVD-SiC material, during torsion testing, but some do not. To elucidate how and where cracks can initiate and propagate in the torsion joint specimens, finite element analyses of these specimens subjected to torsion were performed using a continuum damage mechanics (CDM) model previously developed at PNNL for elastic materials for which any nonlinearity in stress/strain response is due solely to damage and not to other irreversible processes such as plasticity [3]. The CDM model was implemented in the ABAQUS® finite element code via user subroutines. Comparative analyses of the torsion joints using ABAQUS® and the damage model were conducted considering typical mechanical properties of CVD-SiC and different mechanical behaviors of the joint material manifested through the assumed stress/strain responses up to failure. Additionally, since SiC/epoxy and steel/epoxy joints were used to validate the miniature torsion specimen design, a CDM elastic-plastic model was added to this analysis and those results are presented.

Model Formulation

Approach

This section summarizes the damage model and method for predicting crack initiation and propagation [3-5] in the joined CVD-SiC or steel material together with a thin joint region consisting of either Ti_3SiC_2/SiC of varying modulus and strength or a hypothetical brittle epoxy and an elastic-plastic epoxy. Considering damage in an elastic and damageable material, for which any nonlinearity in stress/strain response is due solely to damage and not to other irreversible processes, can be described by a scalar variable, D, that can be related to the microcrack density or microcrack volume fraction, or simply a parameter to

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phenomenologically quantify the level of damage accumulation in the material [4]. Damage affects the material stiffness according to a stiffness reduction law. Using the concepts of thermodynamics of continuous media [4, 6], a thermodynamic potential is defined to derive the constitutive relations and the thermodynamic force associated with the damage variable. This damage model uses the density of the elastic deformation energy as the thermodynamic potential that provides a coupling between damage and elasticity. A damage criterion dependent on a damage threshold function is defined and the damage evolution law is obtained. Damage evolves with the deformation according to the damage evolution law until a critical (saturation) state at which $D = D_{cr}$ $(0 < D_{cr} < 1)$ and failure occurs. D_{cr} is small for brittle materials, and this is the case for ceramic materials studied in this work. In this work, failure at damage saturation ($D = D_{cr}$) leading to crack initiation and propagation is modeled by a vanishing finite element technique [7] that reduces the stiffness and stresses of the failed element to zero [3, 8].

As discussed in Refs. [9, 10] miniature torsion joints were made use Araldite AV119 epoxy between CVD-SiC and a 316-grade stainless steel. AV119 was used to bond these materials after acetone and ultrasonically cleaned surfaces were prepared. The epoxy was cured for 1 h at 130°C [9]. The torsion tests for these samples were performed in the same manner as all the other torsion testing. In addition, simple compressions tests were performed [10] on cylinders of cured AV119 epoxy to establish the mechanical properties of this toughened adhesive material [11, 12]. Materials such as 316SS and AV119 epoxy exhibit pronounced nonlinear behaviors controlled by plasticity and damage. Therefore, an elastic-plastic damage description is used in this work to model the nonlinear responses of these materials to monotonic loading up to failure. Specifically, the model used here is from a model used by Nguyen and Kunc [13] that describes the elastic-plastic damage behavior of a thermoplastic matrix in a long-fiber thermoplastic composite. In this model, the modified Ramberg-Osgood relation captures the material nonlinear stress-strain response:

$$\bar{\varepsilon} = \frac{\bar{\sigma}}{E\,(1-D)} + \frac{\sigma_0}{E}\left(\frac{\bar{\sigma}}{\sigma_0(1-D)}\right)^n = \frac{\tilde{\bar{\sigma}}}{E} + h\,\tilde{\bar{\sigma}}^n \tag{1}$$

where D is the isotropic damage variable, $\bar{\sigma}$ and σ_0 are the equivalent and reference stresses, respectively. The hardening h is given by $h = \sigma_0^{1-n}/E$ where E and n are the elastic modulus and power-law exponent. The "tilde" symbol denotes an effective quantity based on the principle of strain equivalence [14]. The equivalent stress can be expressed in terms of the equivalent plastic strain as:

$$\bar{\sigma} = (1-D)\,k\,(\bar{\varepsilon}^{\mathrm{p}})^{1/n} \tag{2}$$

where $k = (1/h)^{1/n}$ is the hardening coefficient. Using the deformation theory of plasticity and assuming proportional loading, an evolution law for D is sought in terms of stress and plastic strain quantities. To this end, we use the Lemaitre-Chaboche three-dimensional damage model in deformation for isotropic hardening materials [15] that expresses the damage variable increment in terms of the equivalent plastic strain increment as:

$$dD = \frac{D_{\mathrm{c}}}{\bar{\varepsilon}_{\mathrm{p}}^{\mathrm{R}} - \bar{\varepsilon}_{\mathrm{p}}^{\mathrm{D}}}\left(\left[\frac{2}{3}(1+\nu) + 3(1-2\nu)\left(\frac{\sigma^{\mathrm{h}}}{\bar{\sigma}}\right)^2\right] d\bar{\varepsilon}^{\mathrm{p}}\right) \tag{3}$$

where $\bar{\varepsilon}_{\mathrm{p}}^{\mathrm{D}}$ and $\bar{\varepsilon}_{\mathrm{p}}^{\mathrm{R}}$ are the equivalent plastic strains at damage initiation and at rupture, respectively, and D_{c} is the value of D at rupture. ν is Poisson's ratio, and σ^{h} the hydrostatic stress.

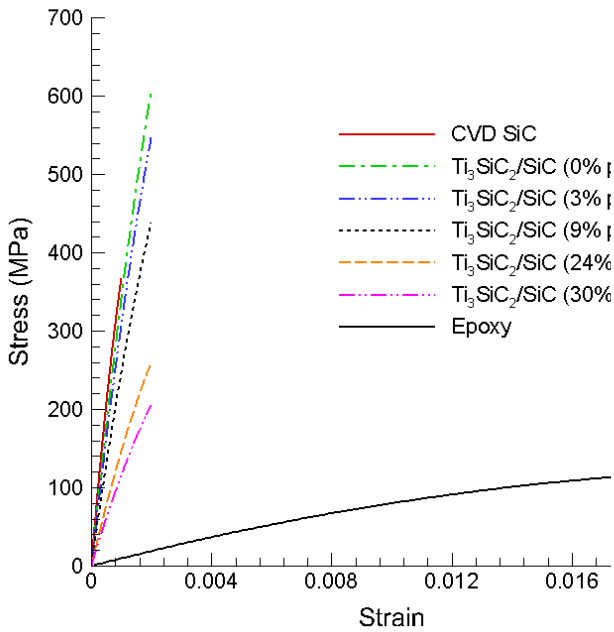
This elastic-plastic damage model was implemented in ABAQUS via user subroutines to describe the constitutive behaviors of the AV119 joint [12] and of the joined 316SS material [16] in the ABAQUS analyses of torsion specimens. Figs. 1b and 1c show the uniaxial stress/strain curves of 316SS and AV119 that are well captured by this elastic-plastic damage model.

Results

Model Results

The damage models are implemented in ABAQUS® as a finite element analysis of the miniature torsion joint specimen. In order to investigate specimen failure for different types of joints, different material properties of the joints were considered and are reflected through the assumed stress/strain responses up to failure in the damage models. In addition, typical mechanical properties of CVD-SiC and nominal steel (316SS) as the joined halves in the experimentally observed range were assumed. Figure 1 and Table 1 present the mechanical properties assumed in this parametric study. There are 5 different behaviors (denoted by case study numbers 1 through 5) considered for the Ti_3SiC_2/SiC composite joint differentiated by their calculated modulus and assumed failure strength. In addition, a similar analysis was performed for two epoxy joined CVD-SiC and steel specimens. The damage variable value at saturation was taken to be 0.2 for all the ceramics while it was considered to be 0.4 for the brittle epoxy (case 6) leading to an epoxy strength of 120 MPa and failure strain of 0.02 and 0.48 for an elastic-plastic epoxy (AV119, case 7) with a strength of 80 MPa at 0.05 failure strain [9, 10, 12].

Damage analyses were conducted for all the torsion joint specimens made of the simulated materials listed in Table 1, which are based on the calculated modulus values for the various joints with differing amounts of porosity. The predicted failure patterns for all the studied cases are gathered in Figure 2. Cases 1 and 5 for the Ti_3SiC_2/SiC joint represent the extreme cases for the most dense joint in Case 1 and the least dense joint in Case 5. The failure location changes from within the CVD-SiC joined materials (Case 1) to within the joint plane (Case 5). Cases 2 and 3 represent Ti_3SiC_2/SiC joints made at 30 MPa and 20 MPa, respectively, which are increasingly less stiff than the joined CVD SiC. For both of these cases, failure is predicted to initiate in the joint but then develop into the SiC sample resulting in out-of-plan failure. Case 4 for the 10 MPa Ti_3SiC_2/SiC joint is now only about 1/3 as stiff as the CDV-SiC and the simulation indicates a mixture of failure within the joint and within the sample. Experimentally, these 10 MPa joints sometimes fail within the joint and sometimes within the CVD-SiC. Case 5 is predicted to fail within the joint and experiments confirm this failure mode. The brittle epoxy joint (Case 6) also always exhibits in-plane failure.



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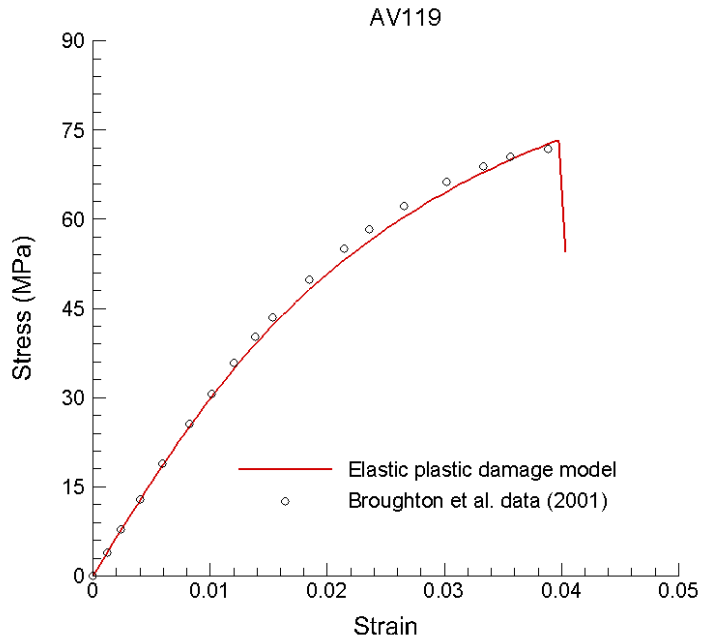

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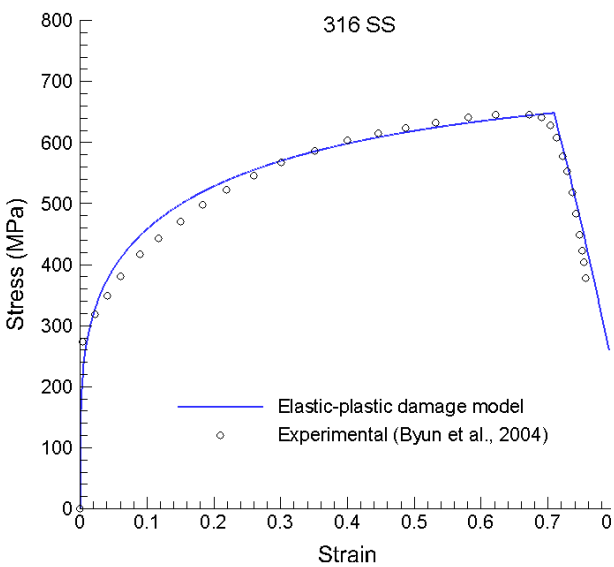


(b)

Figure 1. Uniaxial stress/strain responses considered for (a) an elastic damage model for CVD-SiC and different types of joint material, including a brittle epoxy, (b) an elastic-plastic damage model for 316SS [16] and (c) an elastic-plastic damage model for AV119 epoxy [12]. See Tables 1 and 2 for model parameters.

Table 1. Mechanical properties of the CVD-SiC and joint material assumed for the analysis.

Material	Case Study No.	Elastic Modulus (GPa)	Poisson Ratio	Strength (MPa)	Failure Strain	Damage Variable Critical Value
CVD-SiC	–	460	0.2	368	0.001	0.2
316SS	–	193	0.3	645	0.62	0.7
Ti_3SiC_2/SiC (0% porosity)	1	380	0.2	608	0.002	0.2
Ti_3SiC_2/SiC (3% porosity)	2	343	0.2	548	0.002	0.2
Ti_3SiC_2/SiC (9% porosity)	3	275	0.2	440	0.002	0.2
Ti_3SiC_2/SiC (24% porosity)	4	163	0.2	260	0.002	0.2
Ti_3SiC_2/SiC (30% porosity)	5	129	0.2	206	0.002	0.2
Epoxy (Brittle)	6	10	0.3	120	0.02	0.4
Epoxy 2 (AV119)	7					

Table 2. Parameters of the elastic-plastic models identified for 316SS and AV119.

Materials	E (MPa)	s_0 (MPa)	v	n	$\bar{\varepsilon}_p^D$	$\bar{\varepsilon}_p^R$	D_c
316SS	193000	150	0.3	4.3	0.02	0.42	0.7
AV119	3200	110	0.34	3	0	0.01	0.45

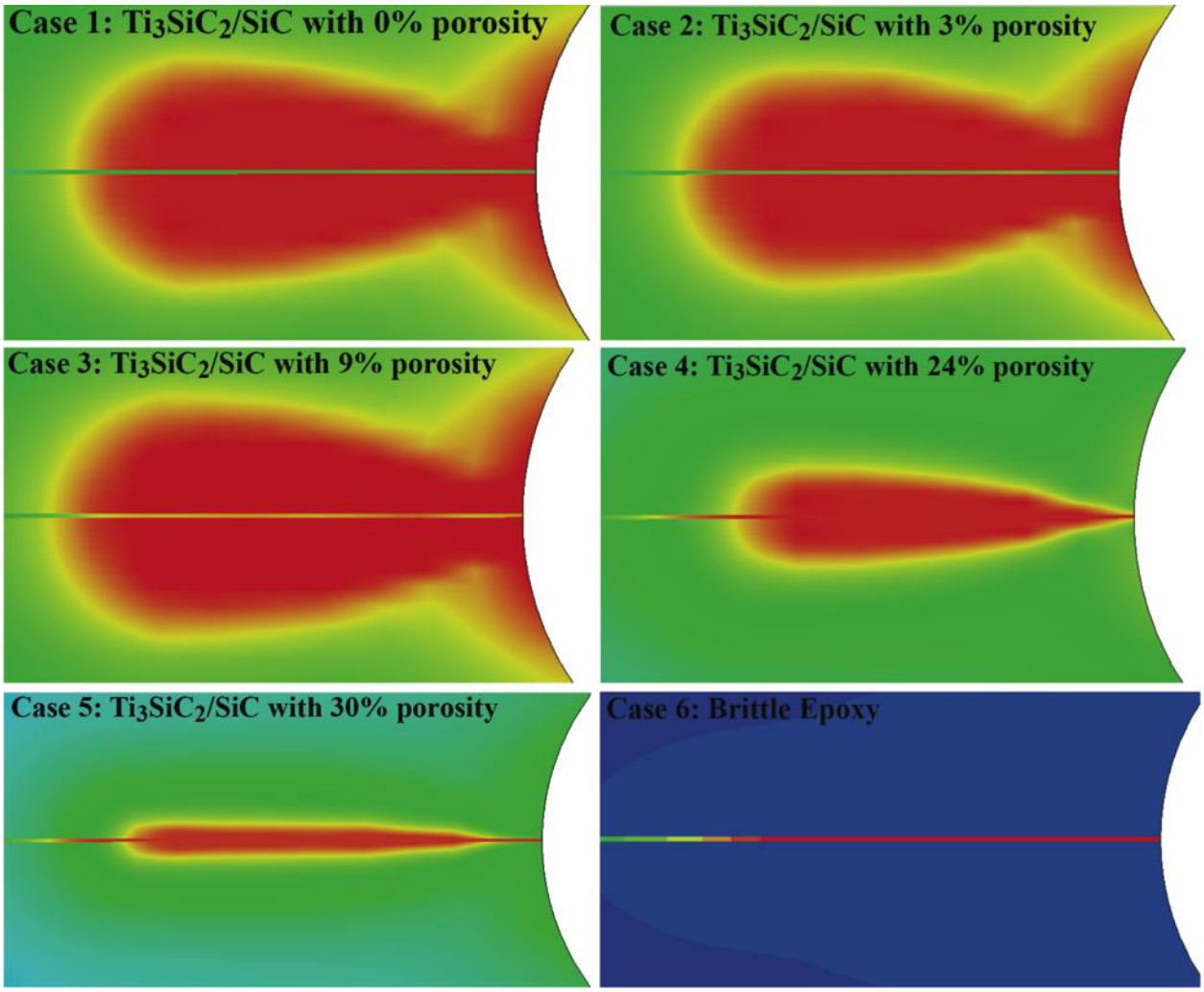
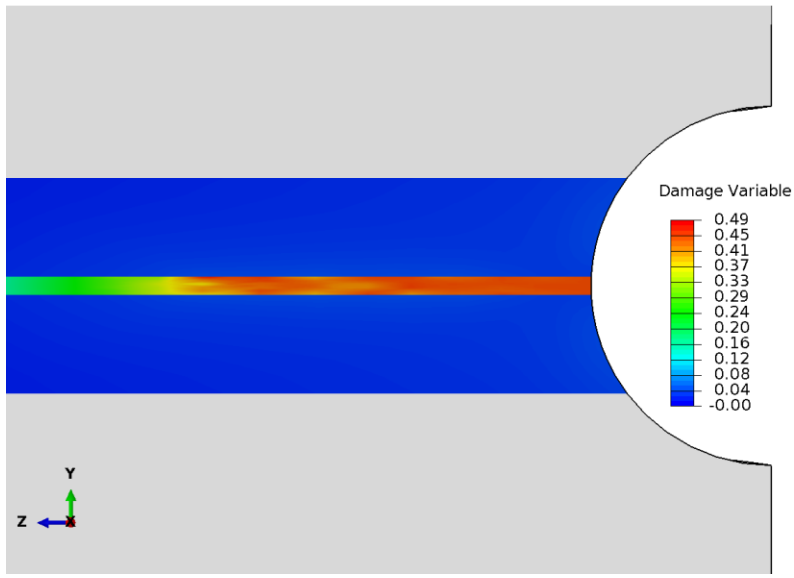


Figure 2. Predicted fracture patterns (red regions) using an elastic damage model for the torsion joint specimens made of different joint materials with mechanical properties listed in Table 1. Cases 1, 2, and 3 fail within the CVD-SiC base material (out-of-plane), while case 4 sometimes fails within the joint . Case 5 always fails in the joint region. Case 6 shows results from the brittle epoxy simulation, which also fails within the joint without exception.

As recognized by Ferraris et al. [10] the toughened adhesive epoxy AV119 is not a brittle material but behaves as an elastic-plastic material and, therefore, must be treated accordingly. Figure 1 and Table 2 together with the elastic-plastic damage model provide the necessary tools to address this issue. In addition to using an elastic-plastic response, the joint thickness in the model was modified to more closely simulate the work performed in Torino. Figure 3 shows the predicted failure locations for a 50-µm thick AV119 joint between CVD-SiC and 316SS. The CVD-SiC is treated elastically as before but in this case the AV119 and 316SS are treated using the elastic-plastic model developed here. The model results validate what the torsion testing observed, namely, that the torsion specimens fracture in the plane of the joint when bonded using AV119 adhesive epoxy regardless of the specimen material.



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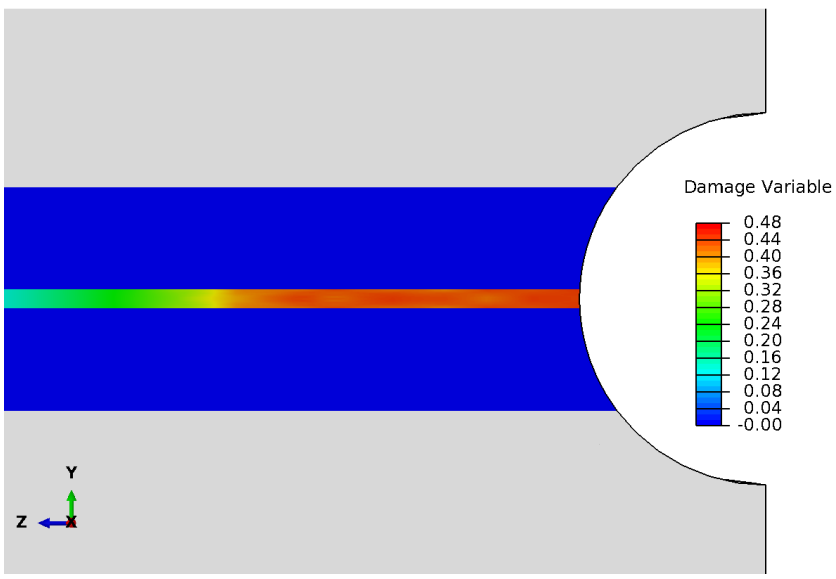


(b)

Figure 3. Predicted fracture patterns using an elastic-plastic damage model for the AV119 adhesive epoxy and for 316SS. Shown in (a) is the predicted fracture for CVD-SiC joined with AV119 where the epoxy is elastic-plastic and the SiC is elastic. Shown in (b) is the case for both materials obeying the elastic-plastic damage model for 316SS joined with AV119 epoxy. In all cases the failure occurs within the epoxy joint.

Discussion

Model Predictions and Comparisons

The damage models were created to help understand the fracture results from the torsion specimens that exhibited non-planar fracture that was not truly reflective of joint properties. Rather, the literature refers to this data as “torsional shear resistance” [1, 2, 17-20] when the torsion specimen fails in the base material, or out-of-plane. The damage model must be able to simulate the stress-strain curves for the constitutive materials; otherwise the model would not be reasonable. The curves shown in Fig. 1 using the data in

Tables 1 and 2 capture the material elastic constants as well as the failure strengths and are very reasonable assumptions. The accuracy of the damage modeling is predicated on the accuracy of the stress-strain data and, even though this model data is not completely precise, the expected results from carefully applying the model are expected to show the correct trends.

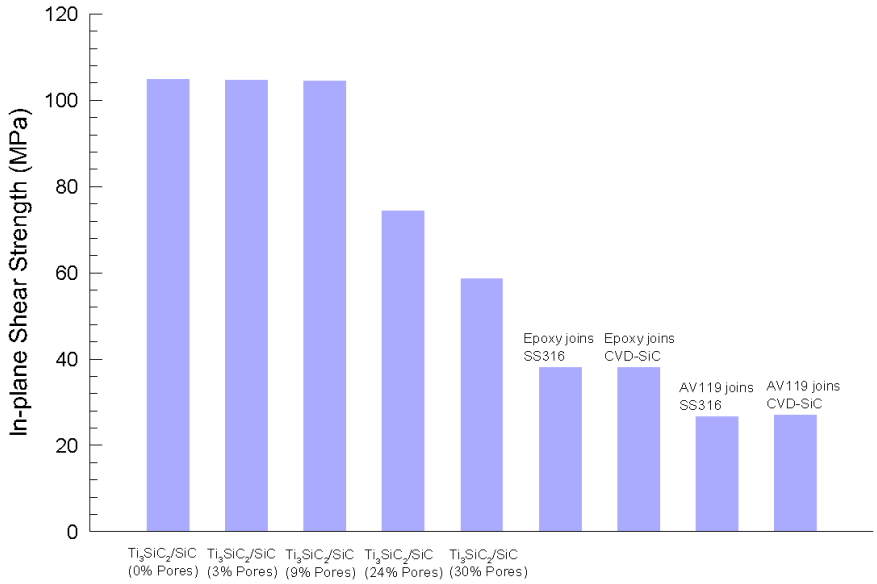
The models, both the elastic and elastic-plastic methods, capture the key observation, namely that there is a transition from planar to non-planar fracture over a range of elastic moduli and strength values. High strength and high moduli materials are predicted to fail out-of-plane and within the base material, whereas much lower modulus and lower strength epoxy (compared to CVD-SiC and 316SS) fails in plane. Intuitively, it is anticipated that low modulus epoxy will behave differently compared to high modulus Ti_3SiC_2/SiC in terms of load sharing with the CVD-SiC base material. In fact, one thought (gedanken) experiment is to imagine the entire miniature torsion specimen machined from a single piece of CVD-SiC and then to try to predict where it will fail. Probabilistic brittle fracture mechanics predicts that it will fail somewhere in the specimen that contains a combination of the largest flaw and the highest tensile/shear stresses, which will not necessarily coincide with the central plane of the torsion specimen. Thus, a high strength, high modulus joint may not fail in the plane of the joint either. As shown in Fig. 2 load sharing with the CVD-SiC forces a majority of the damage to occur within the base CVD-SiC material and failure is predicted to occur out-of-plane of the joint.

However, this load sharing is a function of the modulus difference between the joint and base material. The model predicts a high degree of load sharing and CVD-SiC damage for a joint modulus greater than about 200 GPa and a minimal amount of load sharing with highly localized (planar) fracture for moduli 100 GPa and lower (Fig. 2). This is in good agreement with the observed experimental data for the joints tested at Torino. In addition, the predicted failure strengths in shear match quite well with measurements from ORNL and Torino [1, 17]. The ORNL data for the unirradiated Ti_3SiC_2/SiC joints indicated a torsional shear resistance value of 117 GPa ± 10 GPa, which agrees well with the model data of 104 GPa [1]. Note that this predicted strength value follows from the CVD-SiC damage model that is determined from the assumed CVD-SiC mechanical properties. Thus, the model predicts that the torsion shear test will fail in the CVD-SiC material and that the torsional shear resistance of the sample will be 104 GPa because that is the predicted shear strength of the CVD-SiC simulated here. This failure stress could be increased if stronger base material was provided. Note that the NITE materials tested in Ref. [1] fail at much higher shear strengths compared to the CVD-SiC and this is attributed to the higher strength of the NITE SiC. However, the main point is that for certain joint material combinations that the torsion test will fail at the shear strength limit of the base material and will not provide information regarding the shear strength of the joint material. This is observed in the torsion testing and is predicted by the elastic-damage model.

The epoxy joined data from Politecnico di Torino is more complex. Results indicate a shear fracture strength of 36 MPa, which agrees well with the model prediction of about 38 GPa[2] for the brittle epoxy material (Case 6 and Fig. 4). In this case, where the epoxy modulus is only a fraction of the CVD-SiC or 316SS the fracture path is in the plane of the joint in the epoxy material. Thus, this test will measure a true shear stress value. However, since AV119 toughened adhesive epoxy is not a linear elastic brittle material, the elastic damage model is not appropriate and an elastic-plastic model was developed based on mechanical property data for AV119 and 316SS as discussed. This model predicts a shear failure strength of 28 MPa for a 50-µm thick joint region of AV119 (Figs. 3 and 4), which is less than the calculated value of 36 MPa[1]. However, Ferraris et al. also report a value of 66 MPa ± 10 MPa for AV119-joined CVD-SiC specimens where the shear strength is calculated using Eq. 2, which is inappropriate as discussed in Ref. [10]; rather it is suggested that this value be reduced by 25 to 30% and a value of 45 MPa is suggested as a more accurate value to report. However, this seems to be an arbitrary choice and the results here suggest that a value less than 30 MPa is more accurate. The elastic-plastic damage model provides that prediction based solely on the accuracy of the assumed mechanical properties of AV119 adhesive epoxy taken from Ref. [12]. Since the strength of AV119 depends on the curing time and temperature, etc., the values determined by the elastic-plastic model might differ from other shear strength datasets. However, as can be seen in Fig. 4b the predicted shear stress curves are nonlinear

[2] Personal Communication from Prof. M. Ferraris of Politecnico di Torino. They used AV119 Epoxy with an elastic modulus of 2.8 GPa and Poisson ratio of 0.4. They obtained in-plane shear failures for all tests and calculated a shear strength of 36 MPa ± 8 MPa.

and the use of linear models cannot accurately capture this behavior [10]. Thus, the approach developed here is a much-improved methodology for analyzing miniature torsion test results in the future.



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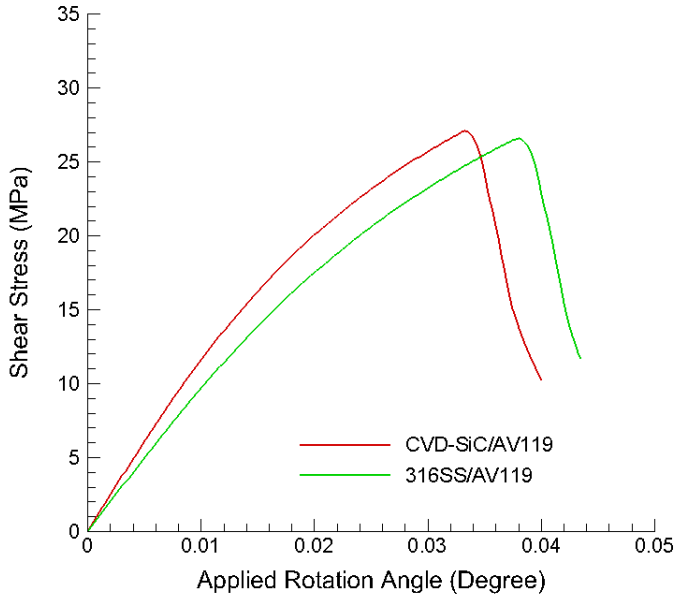

(b)

Figure 4. Graph showing the predicted maximum shear stresses at fracture in (a) for all damage model simulations. Shown in (b) is the predicted evolution of the maximum in-plane shear stresses with applied rotation angle for the elastic-plastic AV119 cases from Fig. 3.

Data Interpretation and Torsion Test Future

Miniature torsion specimens often fail within the joint body or out of the joint plane when the torsion sample base material is a ceramic, such as CVD-SiC, and the joint is strong. This study developed elastic and elastic-plastic damage models that demonstrated that for a wide range of joint moduli and strengths that out-of-plane failure is observed (and predicted) until the joint modulus falls below about 1/3 of the CVD-SiC modulus. The model indicates that out-of-plane fracture is due to load sharing between the joint material and the CVD-SiC causing high shear stresses to develop within the neck region of the torsion sample CVD-SiC (or other ceramic) that surpass the shear strength of the joined material. Since these fractures are probabilistic in nature, there is no guarantee that failures will occur within the plane of a joint for strong, stiff ceramic or glass-ceramic joints. In fact, since the highly stressed volume of the base material is much greater than the volume of the joint material this almost guarantees that for strong, stiff joints failure will occur within the joined ceramic. This finding is documented by many such tests with Ti_3SiC_2/SiC joints that are stronger and almost as stiff as CVD-SiC. Without exception, out-of-plane failure modes were observed for these joints tested in torsion. Joints with intentionally introduced porosity also failed out-of-plane until the joint modulus, which is reduced by the porosity, became less than about 1/3 of the CVD-SiC modulus. At that point in-plane shear failures were observed. However, these results notwithstanding, miniature torsion specimens can still be useful for identifying joint degradation following in-reactor radiation damage by observing either fracture mode changes or observable microstructural changes. The use of these specimens for true joint shear strength measurements is problematic, however. The elastic and elastic-plastic damage models appear to be useful methods that can provide valuable insights into the fracture behavior of the miniature torsion samples.

Future Work

The in-reactor miniature torsion sample irradiation results from ORNL display a failure mechanism that is not included in the model yet, namely, the failure of the joint/CVD-SiC interface. The model assumes a strongly bonded interface between the joint and CVD-SiC and no evolution of that bond is allowed. Future model implementations will treat the interface as a separate material region with an identifiable strength.

Acknowledgements

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