21st International Conference on Composite Materials
Xi'an, 20-25th August 2017

# PREDICTING THE EFFECT OF TEMPERATURE ON MATRIX CRACKING IN THERMOSET COMPOSITES USING A STRAIN INVARIANT APPROACH

Akhila Mukkavilli[1], Garth Pearce[2], Nayeem T. Chowdhury[2] and Alan Crosky[1]

[1] School of Materials Science and Engineering, UNSW Sydney, Australia
[2] School of Mechanical and Manufacturing Engineering, UNSW Sydney, Australia

**Keywords:** Temperature effects, Onset Theory, dilatational invariant, distortional invariant

## ABSTRACT

For a failure theory to be applicable to the general case, it is important to consider the effects of temperature on the material. One of the main proposed advantages of the Onset Theory, a theory that predicts the onset of failure in polymer matrix composites, is that it explicitly accounts for the effects of temperature on matrix failure initiation, an area which has previously not received much attention in the literature. One prediction of the Onset Theory is that the critical dilatational invariant – which governs volumetric failure – should be sensitive to temperature. An analytical model based on the volume expansion behaviour of resin as a function of temperature was developed in order to predict the onset of failure in fibre reinforced composites at various test temperatures and over a range of off-axis fibre angles, within the Onset Theory framework. Using the simplifying assumption of a constant coefficient of thermal expansion (CTE), the model was set up and predicted the overall failure trend as a function of temperature and fibre angle well. The model indicates that the effects of temperature are quite significant, particularly at more extreme temperatures, and a non-linear approach is required.

## 1 INTRODUCTION

Failure in fibre-reinforced composites is a complex, multiscale process and there is still a need to develop a widely applicable failure theory. For a failure criterion to be applicable to the general case, it must have a basis in physical mechanisms.

Gosse and Christensen [1] recognised the need for this and developed the Strain Invariant Failure Criteria, also known as the Onset Theory. The theory is intended to predict the onset of irreversible damage in constrained polymers in fibre reinforced polymer composites. The theory is based on physical material properties in the form of strain invariants, the critical dilatational invariant (the first invariant of strain) and the distortional strain invariant (the equivalent strain, a function of the second invariant of the strain deviator tensor). The theory stipulates that composite performance is governed by two co-existing but non-interacting failure modes corresponding to the invariants –dilatational failure (volume change) and distortional, shear dominated failure (shape change) [1]. Further, separate failure modes are assigned for each constituent. In this work, only matrix failures are considered.

The Onset Theory model employs a micromechanical dehomogenisation technique that calculates strains at the constituent level and then enhances them to the macroscopic scale. This allows for a more accurate approximation of the true strain field in the composite. One feature of Onset Theory approach is that it explicitly accounts for thermal effects on the initiation of matrix failure by considering the elastic strain, which is a combination of the applied mechanical and thermal strains.

A strong support of the Onset Theory having physical basis is that accurate predictions with excellent agreement have been independently generated from the dehomogenisation technique as well as by molecular dynamics simulations [1, 2].

Observations, as well as evidence from molecular dynamics simulations of polymers has suggested that the critical dilatational invariant should be sensitive to temperature, whereas the critical distortional strain invariant is seemingly independent of temperature [3]. A key test of the validity of the Onset Theory's application to the general case can thus be examined by how well it captures any effects of temperature.

The aims of this work were to develop an analytical model based on resin properties capable of predicting the effects of temperature on the critical dilatational invariant, and failure.

## 2 MODEL GENERATION AND INPUTS

The model developed in this work is based on the volume expansion behaviour of resin as a function of temperature. Observations and independent evidence from molecular dynamics simulations show that the critical dilatational invariant should be sensitive to temperature following the trend in Fig. 1[4]. This is anticipated because resin undergoes some volume 'compaction' upon cooling below the glass transition temperature (Tg) and this elastic dilatational contraction is directly related to the thermal contraction. Therefore, it is expected that as temperature decreases, the critical dilatational invariant increases and the relationship described in Equation (1) is observed.

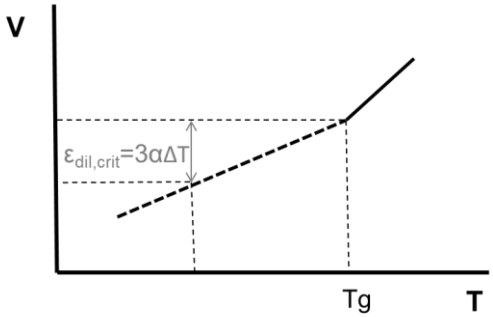


Figure 1: Volume expansion of a resin as a function of temperature.

$$\varepsilon_{crit,dil} = \varepsilon_{crit,dil,RT} + 3\alpha\Delta T \tag{1}$$

Some authors [1, 5] have described the Onset methodology in detail. To summarise, the standard approach for extracting the critical dilatational and distortional invariants is by using a dehomogenisation technique based on micromechanical enhancement factors in Equation (2), in conjunction with off-axis tension testing. Pipes and Gosse [6] prescribed this set of off-axis tests that cover the range of distortional and dilatational driven failures, where the 10° off-axis test gives the critical distortional invariant for the matrix and the 90° off-axis test produces the critical dilatational invariant for the matrix. The three-dimensional failure envelope is shown in Fig. 2. Angles between 10 and 90° change from strongly distortional to dilatational driven failures. Further, angles of approximately 20° to 30° are expected to be on the cusp of both failure surfaces shown in Fig. 2. It is conceived that with a change in temperature, the threshold of this cusp could also move.

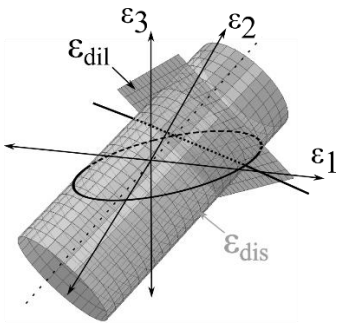


Figure 2: The Onset Theory failure envelope in 3-D space [7].

The micromechanical enhancement procedure has been described in detail in literature [8, 9] and is based on Equation (2).

$$\varepsilon_i^m = M_{ij}^m \bar{\varepsilon}_j + A_i^m \Delta T \tag{2}$$

The aims of this model were to predict the onset of failure in off-axis tests at various temperatures,

without the need for an excessively large experimental test matrix. Since the onset and ultimate states of failure occur simultaneously in off-axis tests [10], the critical invariants can be extracted concurrently, usually by measuring the axial failure strain. Thus, there is a need to approximate the axial failure strain that produces either the critical dilatational or distortional invariant for a given temperature. However, due to the complexity of the calculation, it is not a simple back-calculation.

### 2.1 Material Properties, Inputs and Assumptions

To accurately predict the behaviour of the composite coupon, a consistent set of materials properties is required for both the micromechanical modelling, the continuum simulation and the predictive model. Table 1 shows the material properties for the T300/CYCOM970 unidirectional prepreg system.

| Property | Carbon fibre/epoxy prepreg (T300/CYCOM970) |
|---|---|
| FVF | 0.6* |
| $E_{11}$ (GPa) | 135* |
| $E_{22}$ (GPa) | 7.5‡ |
| $E_{33}$ (GPa) | 7.5‡ |
| $G_{12}$ (GPa) | 3.5* |
| $G_{23}$ (GPa) | 2.76¤ |
| $G_{13}$ (GPa) | 3.5 |
| ν12 | 0.25¤ |
| ν23 | 0.45¤ |
| ν13 | 0.25¤ |

*Measured with high confidence.
‡ Measured with moderate confidence.
¤ Obtained from literature, low confidence.

Table 1: Material properties for selected carbon fibre/epoxy prepreg system (T300/CYCOM 970).

The critical invariants at room temperature are obtained from experimental data, and can simply be implemented into the model as constants. The other elements of Equation (2) are taken from micromechanical modelling, which leaves only the macroscopic elastic strain tensor (the combination of the mechanical and thermal elastic strains - usually obtained from experiment), requiring approximation. To do this, an idealised continuum simulation of a long, thin specimen is generated to capture the behaviour in an evenly distributed strain field, devoid of edge effects. A macroscopic strain probe at the centre of the specimen is extracted for each off-axis fibre angle and used as a 'strain multiplier' to obtain a more realistic strain profile for each off-axis test.

It is then possible to approximate the failure strain by running through the forward-calculation with an initial approximation for the failure strain, and increasing this in small increments until one of the critical properties is met, and failure has occurred. The critical invariants are calculated based on Equations (3) and (4), and a further constraint is put on the critical dilatational invariant as per Equation (1).

$$\varepsilon_{\text{dil}} \equiv J_1 = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 \tag{3}$$

$$\begin{aligned}\varepsilon_{\text{dis}} \equiv \sqrt{J'_2} = \sqrt{\frac{J_1^2}{3} - J_2} &= \sqrt{\left\{\frac{1}{6}\left[\ \varepsilon_{xx} - \varepsilon_{yy}\ ^2 + \ \varepsilon_{yy} - \varepsilon_{zz}\ ^2 + \ \varepsilon_{zz} - \varepsilon_{xx}\ ^2\right] + \ \varepsilon_{xy}^2 + \varepsilon_{yz}^2 + \varepsilon_{zx}^2\ \right\}} \\ &= \sqrt{\left\{\frac{1}{6}\left[\ \varepsilon_1 - \varepsilon_2\ ^2 + \ \varepsilon_2 - \varepsilon_3\ ^2 + \ \varepsilon_3 - \varepsilon_1\ ^2\right]\right\}}\end{aligned} \tag{4}$$

## 3 MODEL PREDICTIONS

### 3.1 A Linear Predictive Model

The model was implemented to create a failure surface which includes the predictions of failure strain and the corresponding failure mode as a function of both temperature and off-axis fibre angle (θ), as shown in Fig. 3.

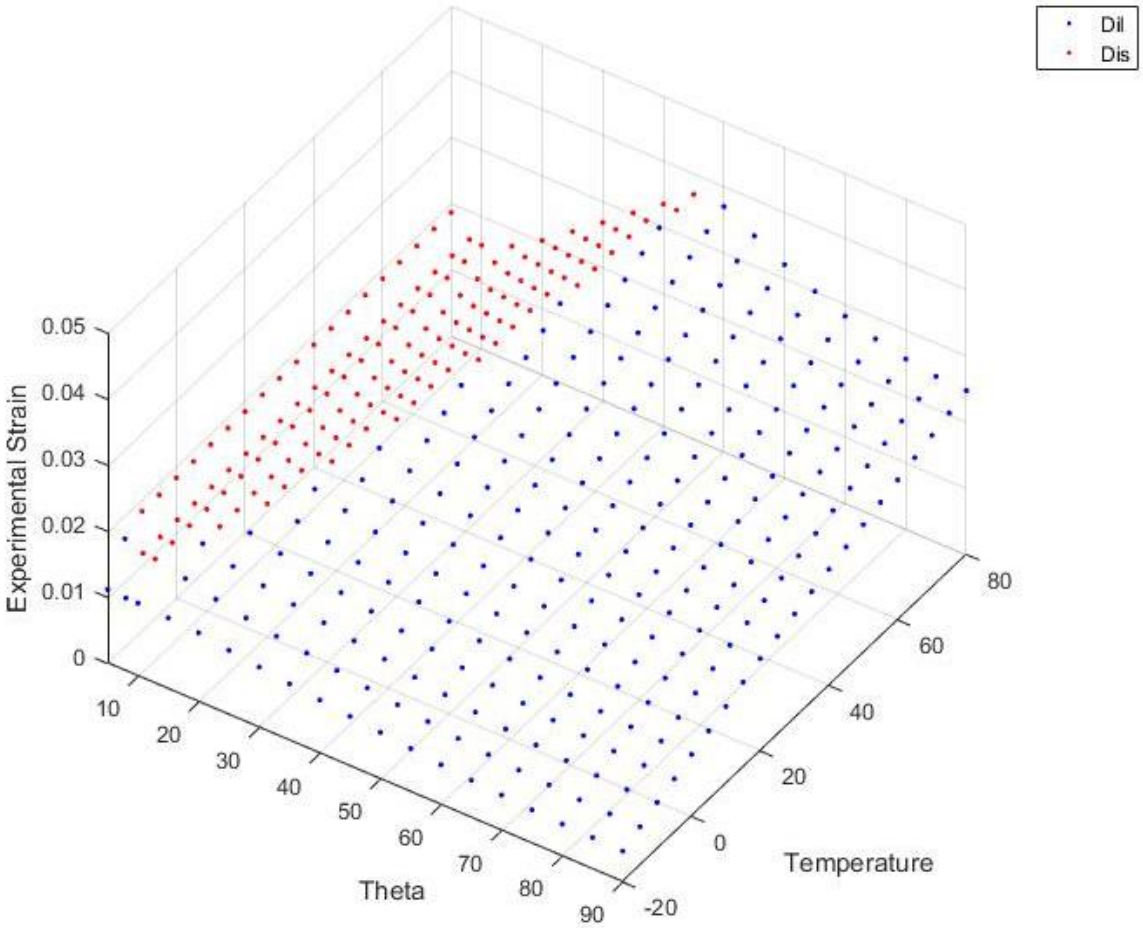


Figure 3: Failure surface showing change in failure mode as a function of temperature and off-axis fibre angle.

For all off-axis fibre angles, increasing test temperature results in an increase in axial failure strain. This is expected as fibre-reinforced composites become more brittle at lower temperatures. However, the model predicts that this effect is more pronounced at mid-range angles between approximately 30-50°.

The model predicts that for the entire temperature range studied, the 90° test will remain strongly dilatational, while the mid-range angles undergo a transition between dilatational and distortional failure over a wide temperature range. For example, a 45° test is expected to change from a strongly dilatational failure at room temperature to being on the cusp of distortional failure at higher temperatures (~75-80°C). The 30° test is expected to change from a dilatational failure at low temperatures to a distortional failure at temperatures slightly above room temperature. Furthermore, for angles below approximately 20°, the failure mode appears to change from strongly distortional failures to dilatationally driven failures at temperatures below 0°C.

To check the model, some preliminary off-axis tension experiments were conducted on rectangular coupons, at various temperatures and the difference between the average experimental failure strain and the predictions of particularly critical cases are given in the table below.

| Off-axis angle | Temperature | Average Strain at Failure (με) | Prediction (με) | Dilatational or Distortional Failure (Predicted Mode) | Variation (%) |
|---|---|---|---|---|---|
| 90° | Low | 9800 | 4700 | Dil (Dil) | -52 |
| 90° | Room | 12400 | 14000 | Dil (Dil) | 20 |
| 90° | Elevated | 15000 | 23900 | Dil (Dil) | 59 |
| 45° | Room | 21600 | 23900 | Dil (Dil) | 11 |
| 45° | Elevated | 31500 | 37100 | Dil (Dis) | 18 |
| 30° | Room | 29000 | 26900 | Dil (Dil/Dis cusp) | -7 |
| 30° | Elevated | 34000 | 26900 | Dis (Dis) | -21 |
| 20° | Low | 14000 | 10500 | Dil (Dil) | -25 |
| 20° | Room | 21300 | 20200 | Dis (Dis) | -5 |

Table 2: Model predictions based on constant CTE case.

It is observed from the experimental work that the model well predicts the overall trends. The experiments showed that a low angle off-axis test generated a higher failure strain than a high angle test, as was predicted. It was also observed that the failure strain increased with temperature over all fibre angles, and the sharper increase in failure strain at elevated temperatures for midrange angles was correctly predicted. In particular, the model well predicted the failure trend at room temperature, with the 30° test having the highest failure strain, followed by the 45°, 20° and 90° tests.

The simplifying assumption in this model is that a constant resin CTE was used. It is known that this material property, along with other elastic properties, changes with temperature. From rudimentary analysis of a fibre in a resin unit cell undergoing cooling, it is expected that a carbon fibre is far less susceptible to thermal contraction compared to the surrounding matrix. If it undergoes any thermal contraction, this would be at a much slower rate than the resin. Therefore, a complex state of stress and strain at the fibre matrix interface could cause an increase in the dilatational invariant, while the resin CTE is thought to contribute more to the overall volume compaction of the system, at least initially. Therefore, to improve the predictions, material non-linearity must be considered.

### 3.2 Extensions for Predicting Failure

The predictive model still requires further refinement of model parameters, particularly for some tests that are on the cusp of dilatational and distortional failure, to better classify the failure mode and capture the magnitude of the effect of temperature more accurately.

Presumably, taking more non-linearity into account by examining the effects of temperature on the elastic material properties may further improve the accuracy of the prediction, work which is currently ongoing. If a non-linear approximation is used, a better schematic representation of Fig. 1 is that shown in Fig. 4, where the volume expansion below Tg follows a somewhat non-linear trend.

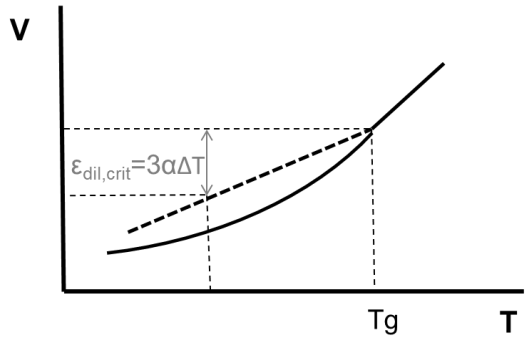


Figure 4: Schematic of a non-linear resin volume expansion as a function of temperature.

In order to better capture the effects of temperature, an updated micromechanical analysis is being conducted in which a representative volume element (RVE) is subjected to non-linear thermal boundary conditions based on dilatometry results, and elastic constants that change as a function of temperature. This new approach is summarized in Fig. 5. Thus, real physical behaviour may be captured more accurately on the micromechanical scale, which can then be enhanced into the macroscopic lamina level using the traditional formulation of Onset Theory, by changing the thermal strain vector to be a function of temperature.

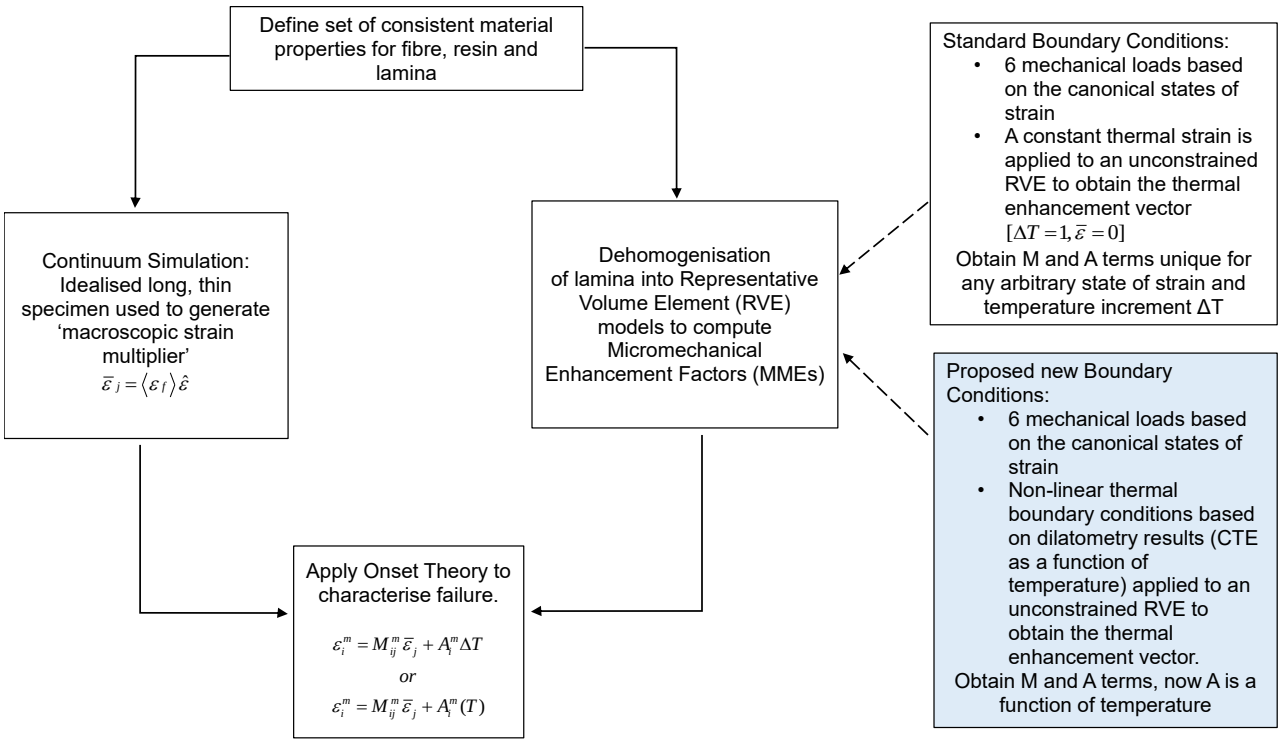


Figure 5: Proposed extension to the Onset procedure to capture the effects of temperature.

## 4 CONCLUSIONS

An analytical predictive model based on volumetric expansion was used in the Onset Theory framework to predict the effect of temperature on the critical dilatational invariant, and therefore final failure. Using the simplifying assumption of constant CTE as a preliminary test, the model could predict the overall trend of off-axis tensile failure with temperature, and in some cases predicted the critical failure mode well. The model suggests that the failure behaviour of composites as a function of

temperature is considerably non-linear, therefore more refinement to the assumptions and inputs are needed to gain a more accurate understanding of the effects of temperature – work which is ongoing.

## REFERENCES

[1] J. Gosse and S. Christensen, "Strain invariant failure criteria for polymers in composite materials," presented at the 42nd AIAA/ASME/AHS/ASC Structures, Seattle, Washington, 2001.

[2] S. Christensen, "Using molecular dynamics coupled with higher lengthscale simulations for the development of improved composite matrix materials," presented at the ICCM-17, the 17th International Conference on Composite Materials, Edinburgh, UK, 2009.

[3] L. J. Hart-Smith, "Application of the strain invariant failure theory (SIFT) to metals and fiber–polymer composites," *Philosophical Magazine,* vol. 90, pp. 4263-4331, 2010/11/07 2010.

[4] S. Christensen and R. D'Oyen, "Computational formulation of a new composite matrix," *Scripta Materialia,* vol. 70, pp. 18-24, 1/1/ 2014.

[5] T. D. Tran, "Development of micromechanical modelling procedures using the Onset Theory for failure of composites," PhD, UNSW Australia, 2012.

[6] R. B. Pipes and J. H. Gosse, "An Onset Theory for Irreversible Deformation in Composite Materials," in *ICCM-17- 17th International Conference on Composite Materials*, Edinburgh, 2009.

[7] N. T. Chowdhury, "A novel failure criterion for matrix dominant failure within fibre reinforced polymer composites," Doctor of Philosophy, Faculty of Engineering, Department of Mechanical and Aerospace Engineering, Monash University, 2016.

[8] D. L. Buchanan, J. H. Gosse, J. A. Wollschlager, A. Ritchey, and R. B. Pipes, "Micromechanical enhancement of the macroscopic strain state for advance composite materials," *Composite Science and Technology,* vol. 69, pp. 1974-1978, 2009.

[9] S. H. Lim, G. Pearce, D. Kelly, B. G. Prusty, and A. Crosky, "New Developments in Onset Theory for Onset of Resin Failure in Fibre Reinforced Composites," presented at the 19th International Conference on Composite Materials, Montreal, Canada, 2013.

[10] J. M. Caruthers and G. A. Medvedev, "Nonlinear Viscoelastic Behaviour of Glassy Polymers and Its Effect on the Onset of Irreversible Deformation of the Matrix Resin in Continuous Fibre Composites," presented at the ICCM-17: 17th International Conference on Composite Materials, Edinburgh, 2009.