Characterisation and micromechanical modelling of a temperature dependent hyper-viscoelastic polymer bonded explosive

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Presenter biography

Dr. Joanna Li-Mayer is a postdoctoral researcher at Imperial College London. Her research focuses on the development of computational models to predict the thermo-mechanical behaviour of polymer bonded explosives. She has particular interests in characterisation of non-linear soft solids, damage mechanics, image based computational models and multi-scale methods.

Abstract

Polymer bonded explosives (PBXs) are highly filled binary particulate composites, typically >90% volume fraction. The composites consist of a compliant matrix binder and rigid filler crystals. In order to predict the bulk composite behaviour, the polymer matrix material properties and a suitable constitutive model was determined for use in a multi-scale micromechanical finite element model.

The matrix material was characterized using monotonic tensile tests at room temperature as well as small strain and large strain shear rheometry tests at different temperatures. A temperature-dependent visco-hyperelastic constitutive model combining the use of the Prony series and the Van der Waals potential was used to describe the matrix material behaviour. Material parameters at room temperature were first optimized by minimisation of the error function between the experimental and predicted behaviour (MATLAB, MathWorks). Temperature dependence for higher temperatures was then determined using time-temperature superposition.

A 3D micromechanical finite element model, reconstructed from X-Ray tomographic data, was used for prediction of the composite behaviour. Due to the loss of some filler particles during the image processing and model reconstruction, a hierarchical method was used to incorporate the missing volume fraction.

1. Characterisation of the binder material

Uni-axial monotonic tensile tests were conducted using dumbbell samples under constant true strain rate loading of 0.1, 0.01 and 0.001/s at room temperature, results are shown in figure 1. Simple shear behaviour was also investigate under constant shear strain rate loading of 0.01, 0.1 and 1/s.

1.1. Constitutive material model

The binder material exhibited large strain elasticity and time dependent behaviour. To describe the time and strain dependent behaviour mathematically, the mechanical response can be simply described as a combination of the strain dependent stress function, $\sigma_0(\varepsilon)$, and a time dependent stress function, $g(t)$, where σ is the true stress, ε is the true strain and t is time[1].

$$\sigma(\varepsilon, t) = \sigma_0(\varepsilon) g(t)$$

For hyperelasticity, true stress in uni-axial and simple shear deformation was defined as a function of the stretch ratio, λ,

$$\sigma_o(\lambda) = \frac{\partial W}{\partial \lambda}\lambda$$

$$\sigma_o(\lambda) = \frac{dW}{d\lambda}\frac{d\lambda}{d\gamma}$$

Where *W* is the strain energy function and γ is shear strain. In this work, the Van der Waals strain energy function was used,

$$W = -\mu\left\{(\lambda_m^2 - 3)\left[ln\left(1 - \sqrt{\frac{I_1 - 3}{\lambda_m^2 - 3}}\right) + \sqrt{\frac{I_1 - 3}{\lambda_m^2 - 3}}\right] + \frac{2}{3}a\left(\frac{I_1 - 3}{2}\right)^{\frac{3}{2}}\right\}$$

where λ_m is the the locking stretch constant, μ is the instantaneous shear modulus, *a* is the global interaction parameter and the first invariant defined, $I_1 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2$. The three principal stretch ratios, λ_1, λ_2 and λ_3 are then determined from the stretch ratio under uni-axial loading, assuming the two lateral stretch ratios, λ_2 and λ_3, are equal, giving $\lambda_1 = \lambda$ and $\lambda_2 = \lambda_3 = \frac{1}{\sqrt{\lambda}}$. Whereas in simple shear, the three principal stretch ratios are defined as, $\lambda_1 = \lambda$, $\lambda_2 = 1$ and $\lambda_3 = \frac{1}{\sqrt{\lambda}}$. Finally, the stretch ratio is related to true strain and shear strain by $\ln(\lambda) = \varepsilon$ and $\lambda = \frac{\gamma}{2} + \frac{\sqrt{\gamma^2+4}}{2}$ respectively.

To incorporate the time dependent behaviour, the Prony series was used for the time dependent stress function,

$$g(t) = g_\infty + \sum_{i=1}^{N} g_i e^{(-t/\tau_i)}$$

where g_∞ and g_i are dimensionless coefficients, τ_i are the relaxation time constants.

The hyper-viscoelastic model was implemented in MATLAB and the unknown parameters were determined by using an optimisation algorithm to minimise the sum squared error between the model predicted and experimentally measured monotonic tensile and simple shear behaviour. The fit of the model with optimised parameters to experimental data under monotonic tensile and simple shear loading at room temperature is shown in figure 1.

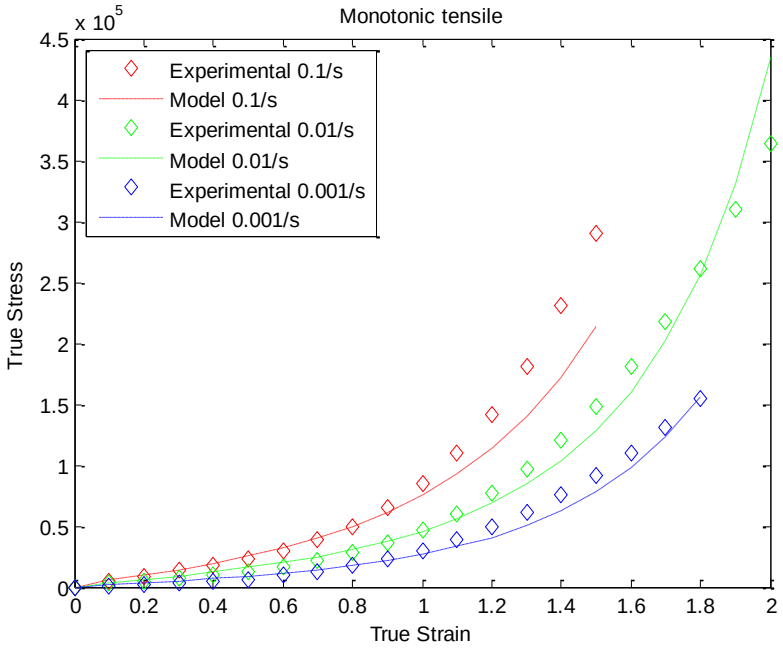

Figure 1 Comparison between tensile experimental and model prediction for the binder at room temperature

The temperature dependent behaviour of the binder was characterised using oscillatory frequency sweeps performed at temperatures of 0, 25, 40, 50 and 60˚C. The isothermal storage modulus curves measured at 0, 40, 50 and 60˚C were then shifted taking 25˚C as the reference temperature to produce a single master curve. The determined shift factors, α_T, allows the temperature dependency of the material to be described by shifting the time constants of the prony series as follows[2, 3],

$$\alpha_T = \frac{\tau_i(T)}{\tau_i(T_{ref})}$$

where T and T_{ref} are the actually and reference temperature in ˚C respectively, τ_i are the relaxation time constants for i=1,2,3…n and g_i are the corresponding elastic modulus for each relaxation time constant. The relationship between the shift factors and temperature was implemented in FE using the Williams-Landel-Ferry equation[4],

$$\log \alpha_T = \frac{-C_1(T - T_{ref})}{C_2 + (T - T_{ref})}$$

where C_1 and C_2 are the Williams-Landel-Ferry constants used to define the relationship.

2. Micromechanical model finite element model

Image data of the composite was obtained at Diamond Light Source, Didcot, UK. Only a small portion of the available 3D image data with a field of view of 263 x 263 x 263 μm was segmented to limit the FE model size. Imaged at a resolution of 0.4 x 0.4 x 0.4 μm/voxel, delineation of the boundaries and the inter-particle matrix region between some of the closer packed fillers was found to be difficult. As a result, the volume fraction of the segmented filler volume fraction was lower than the actual composite filler volume fraction of 90%. The segmented microstructure with a filler volume fraction of 41% is shown in figure 2.

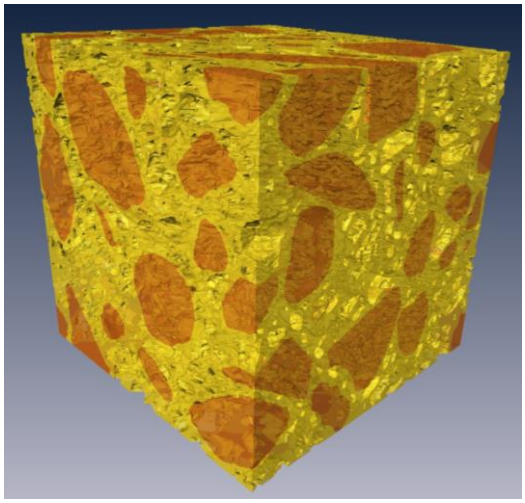

Figure 2 Computer rendering of the segmented microstructure from CT image data at 41% filler volume fraction

2.1. Finite Element model

The geometries of the particles segmented from image data were reconstructed in finite element. Due to the complexity of the particle geometries and close proximity of some of the particles, it was impossible to generate a finite element mesh for the 41% filler volume fraction RVE. As a result, the number of particles reconstructed was reduced to include only 11 of the larger particles, giving a total filler volume fraction of 12%, shown in figure 3. The missing 78% filler volume fraction is accounted for in the model by incorporation into the matrix volume. A Mori-Tanaka analytical solution was used for determining the homogenised material properties of matrix with the missing filler particles[5].

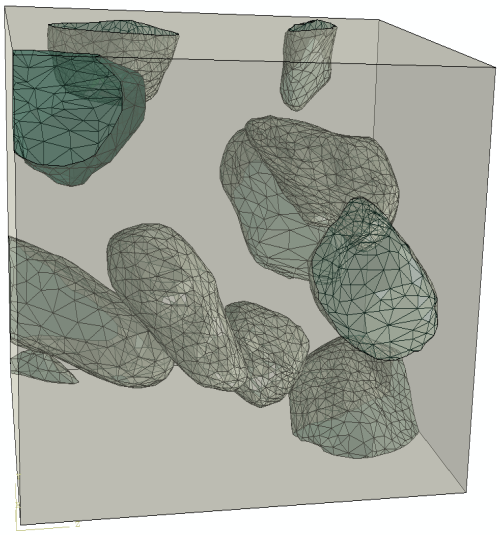

Figure 3 Computer rendering of the FE model with 12% filler volume fraction

The FE model was analysed using the quasi-static implicit solver in Abaqus 6.14 (SIMULIA, Rhode Island, USA). 36k quadratic tetrahedral elements for 3D stress, C3D10, were used for the fillers and 146k quadratic tetrahedral elements with hybrid formulation, C3D10H, were used for the matrix. A tensile strain of 0.01 was applied to the top edge of the RVE at a strain rate of 0.0001/s at 0, 25, 40, and 60˚C, results are shown in figure 4.

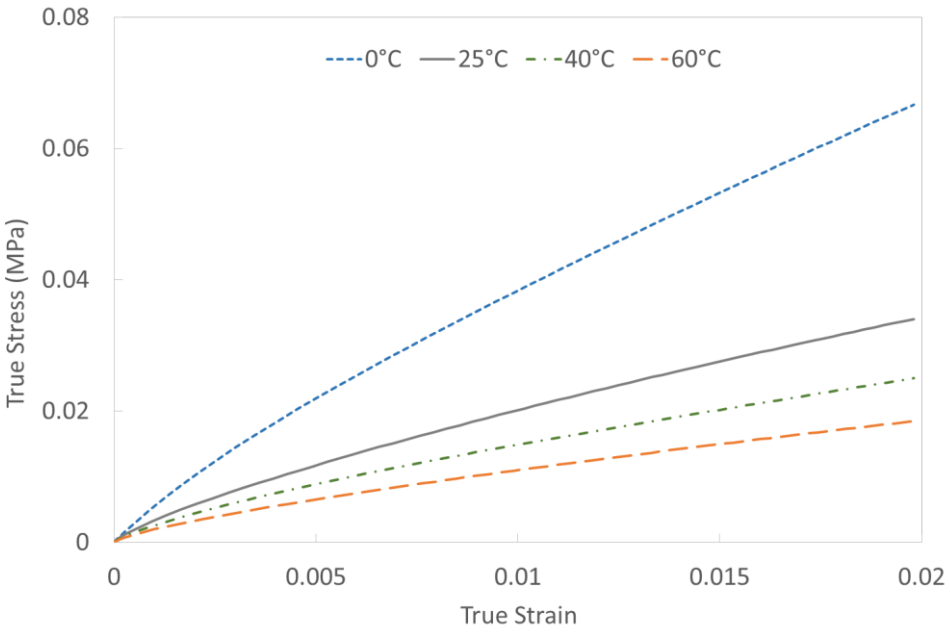

Figure 4 FE model predictions of the 90% filler volume fraction filled composite tensile behaviour under a strain rate loading of 0.0001/s at 0, 25, 40 and 60°C

3. Conclusions

The current FE model is able to predict the tensile behaviour of the 90% filler volume fraction filled composite within the calibrated strain rates and temperatures. To improve the accuracy of the model predictions, work is being carried out to increase the volume fraction of the image reconstructed 3D FE model.

Acknowledgments

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