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Modelling the damage and deformation process in a plastic bonded explosive microstructure under tension using the finite element method

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ABSTRACT

Modelling the deformation and failure processes occurring in polymer bonded explosives (PBX) and other energetic materials is of great importance for processing methods and lifetime storage purposes. Crystal debonding is undesirable since this can lead to contamination and a reduction in mechanical properties. An insensitive high explosive (PBX-1) was the focus of the study. This binary particulate composite consists of (TATB) filler particles encapsulated in a polymeric binder (KELF800). The particle/matrix interface was characterised with a bi-linear cohesive law, the filler was treated as elastic and the matrix as visco-hyperelastic. Material parameters were determined experimentally for the binder and the cohesive parameters were obtained previously from Williamson et al. (2014) and Gee et al. (2007) for the interface. Once calibrated, the material laws were implemented in a finite element model to allow the macroscopic response of the composite to be simulated. A finite element mesh was generated using a SEM image to identify the filler particles which are represented as a set of 2D polygons. Simulated microstructures were also generated with the same size distribution and volume fraction only with the idealised assumption that the particles are a set of circles in 2D and spheres in 3D. The various model results were compared and a number of other variables were examined for their influence on the global deformation behaviour such as strain rate, cohesive parameters and contrast between filler and matrix modulus. The overwhelming outcome is that the geometry of the particles plays a crucial role in determining the onset of failure and the severity of fracture in relation to whether it is a purely local or global failure. The model was validated against a set of uniaxial tensile tests on PBX-1 and it was found that it predicted the initial modulus and failure stress and strain well.

1. Introduction

Particle filled polymer composites can provide economic and technical advantages over other engineering materials. By reinforcing a polymeric matrix with stiffer filler particles the mechanical properties of the composite can be tuned to meet specific requirements by choosing appropriate constituent phases [1].

Numerical studies on the effect of microstructure, arrangement and volume content of hard damageable inclusions in a plastic matrix on the deformation and damage growth has been conducted by Mishnaevsky [2]. He highlighted that particle arrangement does not influence the effective response of the material in the elastic region or at small plastic deformation, however it becomes significant at loads at which the particles begin to fail. The distribution of particles was shown to have significant effects based on their arrangement, with more structured arrangements having higher flow stresses compared to random or skewed/biased arrangements. The effect of increasing size caused a very strong decrease in the strain hardening rate and lead to quicker and earlier damage growth in the composites. Diler and Ipek [3] showed experimentally and numerically that increasing volume fraction and particle size of their Al–SiC_p composites reduces flexural strength, with volume fraction having a more significant effect.

Fu et al. [4] studied the effects of particle size, particle/matrix adhesion and particle loading on composite stiffness, strength and toughness of a range of particulate composites having both micro- and nano-fillers with small aspect ratios. It was shown that composite strength and toughness are strongly affected by all three factors, especially particle/matrix adhesion. This is expected, because strength depends on effective stress transfer between filler and matrix, and therefore toughness is controlled by the

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particle/matrix adhesion. Maloney et al. [5] reviewed previous attempts at experimentally modifying certain parameters such as filler volume fraction, stiffness and size as well as strength of both the filler and matrix to assess the effect each had on the stiffness, strength and fracture toughness of the composite. It is worth mentioning here that conventional particle reinforced composites go up to volume fractions of 50%, due to limits in what can be fabricated, which is significantly lower to that studied here.

Polymer bonded explosives (PBX) are used in a wide variety of civil and military applications such as detonators and solid rocket propellants. The volume of explosive crystals used within PBX can vary from 60% to 95% by mass [6]. The inert binder is used to reduce the shock sensitivity of the explosive and to make it safer to handle. PBX formulations can vary greatly depending on their application. Crystal/filler choices are made based upon sensitivity, energy release and achievable packing density. The matrix/binder material is used to bond these fillers together in a way such that they can achieve their potential. The binder can strongly affect the formability and fracture properties of the PBX.

The small volume of binder material can strongly influence the behaviour of the composite as there is generally a large mismatch in moduli between the stiff crystals and the binder. This binder material enables the composite to deform and absorb energy and it is this that allows the PBX to be prepared and machined to desired shapes and sizes. However it is the quality of the interface which is also a significant concern for manufacturers. Understanding the behaviour of the material on a micro-scale is essential to ensure minimal loss of the filler during processing. Finite element (FE) analysis of these microstructures allows the full-field strain map to be predicted. A knowledge of the strain field inside the filler, matrix and along the particle/matrix interface is essential to predict matrix or particle cracking and debonding between the filler and the matrix. Early works in this area include research such as that of Guild and Young [7] looking into the application of combined numerical and statistical methods to predict the elastic properties of particle filled composite materials. The model, validated against macro-scale experimentation, allowed for improved understanding of the failure process occurring on a micro-scale between glass spheres and the matrix. PBX formulations can vary greatly depending on their application and therefore require individual and unique modelling approaches.

More recently work such as that by Barua and Zhou [6] attempted to simulate large volume fraction grades of PBX. Cohesive zone finite element methods were implemented on a digitised microstructure as well as idealised geometries of particle distributions. Bimodal distributions of particle sizes produced composites with improved mechanical integrity over a monomodal distribution of particles sizes. They also highlighted that failure at the interface was more likely in regions of flat faced particles compared to round ones. Particle debonding in high filled elastomers used in solid propellants was also investigated by Matous et al. [8]. They modelled particle debonding through cohesive laws and determined its effect on the macroscopic mechanical response of the composite through a small strain, multi-scale formulation. The simulations were performed using a packing algorithm, generating a unit cell matching the volume fraction and particle size distribution of the actual composites. Seidel et al. [9] used a finite element code to simulate the mechanical response of LX17. Because of the highly filled nature of the material, Voronoi tessellation was used to represent the explosive crystals. The latter were surrounded by linear viscoelastic cohesive zones that represented the binder matrix. A comparison was made between their simulation results and experimental data. Yan-Qing and Feng-Lei [10] studied PBX9501 composites and employed a similar technique, i.e. the Voronoi tessellation method with a viscoelastic cohesive law at the particle interface. Cracking in the HMX particles was accounted through a tensile crack model and they validated their predictions with experimental data. Finally, purely experimental studies on PBX materials have also been reported in literature, e.g. Liu et al. [11], Drodge et al.[12], Chen et al. [13], Thompson et al. [14], Gee et al. [15], Rae et al. [16]. The work presented here builds on research such as this, developing a method and process for analysing actual microstructures of binary particle filled composites. In real PBX microstructures there are fine particles, which will be present in the binding material accounting for a significant portion of the filler volume fraction. This has previously been accounted for by either expanding or dilating digitised geometries [6], or through using Voronoi tesselated microstructures with viscoelastic cohesive zones. Note that in our method, the matrix and the interface are modelled separately unlike Voronoi tessellation methods. The model presented here is different to the reported literature in that it captures all large particles and models them explicitly, whilst fine particles are accounted for by increasing the stiffness of the matrix material model. This enables very high volume fraction composites to be modelled, compared to the general literature in the area focused on volume fractions below 50% for particulate filled composites. The damage criteria for fracture is also developed here and included within the analysis, allowing the complex damage development process within these particulate composites to be modelled explicitly.

2. Material constitutive laws: development and characterization

2.1. Composite materials

The PBX composition investigated here is referred to as PBX-1. This comprises a KELF800 matrix material, which is a chloro-tri-fluoro-ethylene vinylidene-fluoride co-polymer that exhibits a non-linear viscoelastic behaviour. The filler material is TATB, or triamino-trinitrobenzene, which is assumed to be a linear elastic solid. To guide the development and validate the model, the PBX was tested under uniaxial tension at 2×10^{-3}/s. Cylindrical dumb-bell specimens were cast with a gauge length of 33.2 mm with a constant diameter of 10.2 mm. The densities of TATB and KELF800 are 1.94 g/cm^3 and 2.00 g/cm^3 respectively. The composite contains 95% TATB by mass fraction, equating to a 95.1% volume fraction.

Table 1 shows a summary of the tensile test results. The Young's modulus, E, failure strain, ε_f, and failure stress, σ_f, for each of the three replicate specimens are given. There is a small statistical sample collected here due to the expense, environmental considerations and hazards involved to fabricate and test this type of materials.

A set of images of various magnifications were obtained prior to testing to quantify the particle size distribution visible within the finished product. These are shown in Fig. 1.

The two phases can be identified in the sample images shown in Fig. 1. Obtaining SEM images of this microstructure is a challenge compared to conventional composite materials, due to the smearing effect that is observed during sample preparation. One of the images shown in Fig. 1, Image 3, was selected to generate the finite

Table 1
Raw tensile test data for the composite material.

Sample	ε_f	σ_f (MPa)	E (GPa)
1	0.00174	8.263	7.85
2	0.00161	7.929	8.02
3	0.00189	8.567	7.11
Average	0.00174	8.253	7.66