COMPUTATIONAL MODELLING AND INVESTIGATION OF STRAIN AND DAMAGE SENSING IN MOCK ENERGETIC MATERIALS

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ABSTRACT

The study of the mechanical responses of mock energetic material composites is important for understanding their behavior under various loading conditions. This research objective studies materials composed of sugar grain, a binder region, and voids. Carbon nanotubes can be introduced into the binder regions of these materials to enable damage sensing through observing changes in electrical conductivity. This allows for the detection of cracks or deformities within energetic materials that may affect their performance. Abaqus, a commercial Finite Element Analysis software, is used to determine the Young's modulus of sugar grains to develop a more encompassing model of mock energetic materials. Individual representative volume elements (RVEs) are simulated in a compression test, and the effective Young's modulus is calculated. The experimental effective Young's modulus of the simulated RVEs is known, though the sugar constituent Young's modulus is found by determining the relationship between the sugar and effective Young's modulus. The sugar grain Young's modulus is interpolated to be 714.02 MPa. This value allows for more accurate simulations of mock energetic materials, and will be used in future simulations to study mechanical, thermal, and electrical responses during damage propagation.

INTRODUCTION

This investigation aims to determine material properties of mock energetic materials composites using Finite Element Analysis (FEA) software. The mock energetic materials that are simulated for this analysis are composed of sugar and a binder region. The inclusion of carbon nanotubes (CNTs) in mock energetic materials composites enable damage sensing through observing changes in conductivity of the material.[1] Carbon nanotubes have high electrical conductivity, and when introduced into polymers and composite materials, these composites gain conductive properties. As a result, when damage propagates through a material and breaks these conductive pathways, the conductivity of the material changes.

This investigation is necessary for developing more encompassing models of mock energetic materials. Mock energetic materials have a wide range of applications, including in solid rocket fuel. Typically, solid rocket fuel consists of ammonium perchlorate (the oxidizer), aluminum power, and a binder (such as polybutadiene acrylonitrile, PBN). CNTs can be introduced into the binder region of this material to allow for damage sensing.

The performance of solid rocket fuel is typically quantified by properties such as regression rate and specific impulse. However, properties such as Young's modulus and fracture energy are important variables that should be investigated. During transport, solid rocket fuel can experience damaging loads, and this may result in a change in the fuel's performance. For example, a crack within a fuel grain that is not visible from the exterior can cause a change in the core grain geometry, changing the regression rate. This can be detected through measuring the electrical conductivity of the material. Also, research has been conducted on dynamic loads acting on energetic materials, though further research needs to be conducted in investigating the effects of static loads.

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The materials simulated for this investigation have been tested experimentally to determine their Young's modulus, though the material properties of the sugar within the samples are unknown. Testing sugar grains experimentally using simple tensile or compression testing is difficult, and therefore the following analysis solves the inverse problem of determining constituent material properties. The methods and analysis within this investigation involve modelling compressive simulations of the Representative Volume Elements (RVEs) of the samples and calculating the effective Young's modulus. With this information, and a range of Young's modulus values for sugar, the true Young's modulus of the sugar grains is determined.

Relevance to NASA Mission Directorates

The Space Technology NASA mission directorate focuses on developing technology for the exploration of the moon. The models created in this investigation work towards developing a deeper understanding into mock energetic materials, and therefore solid rocket fuel used for launch vehicles.

In addition, this investigation applies towards the Space Operations mission area of the Human Exploration and Operations mission directorate. Solid rocket fuel enables launch vehicle research and development, that directly applies to the development of technologies for the exploration of humans beyond Earth's atmosphere.

Statics, Structures, and Materials

An understanding of materials and structures is necessary for the discussion of Finite Element Analysis and compression testing. Stress and strain are basic principles used throughout this analysis. Stress is defined as the force that is applied on a material per unit area, and strain is the deformation relative to the initial material dimension.

The 3D constitutive relation relates stress and strain, and can be seen in Equation 1.

$$\begin{pmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ 2\epsilon_{23} \\ 2\epsilon_{13} \\ 2\epsilon_{12} \end{pmatrix} = \begin{bmatrix} 1/E & -\nu/E & -\nu/E & 0 & 0 & 0 \\ -\nu/E & 1/E & -\nu/E & 0 & 0 & 0 \\ -\nu/E & -\nu/E & 1/E & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/G \end{bmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{pmatrix} \quad (1)$$

Some material properties that are discussed within this analysis are Poisson's ratio and Young's modulus. Poisson's ratio is a value that quantifies a material's ability to deform and is defined as seen in Equation 2.

$$\nu = -\frac{\varepsilon_{lateral}}{\varepsilon_{axial}} \quad (2)$$

The constitutive relation simplifies for a compression test where sides are unconstrained (as further described in the Experimental Method section of this report). This reduces the formula to Equation 3.

$$E = \frac{\sigma_{22}}{\varepsilon_{22}} \quad (3)$$

This formula assumes that the material is within the "linear elastic" region, which is when the stress vs. strain curve is linear, as seen in Figure 1. This region is characterized by elastic deformation with no damage. For all discussion within this analysis, the material is assumed to be in the linear elastic region.

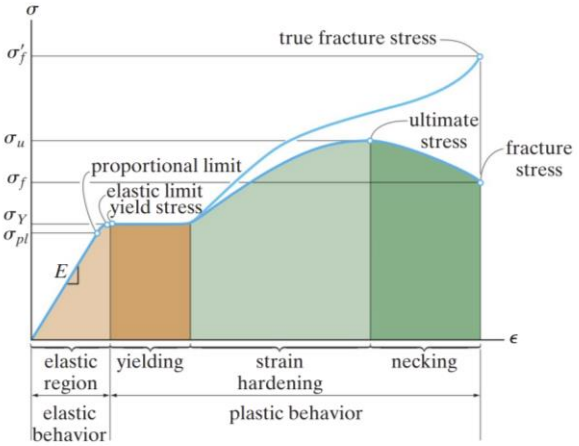

Figure 1. Stress vs. Strain Diagram[2]

Inverse Problem

To properly simulate the mock energetic material RVE's using FEA, the constituent material properties must be known. However, the sugar's Young modulus is unknown. Therefore, computational models are run at various sugar Young's modulus values, effectively creating a set of data points. These data points are then used for interpolation to find an effective Young's modulus of the composite derived from experimental testing (15.72 MPa) along with the corresponding sugar Young's modulus.[3]

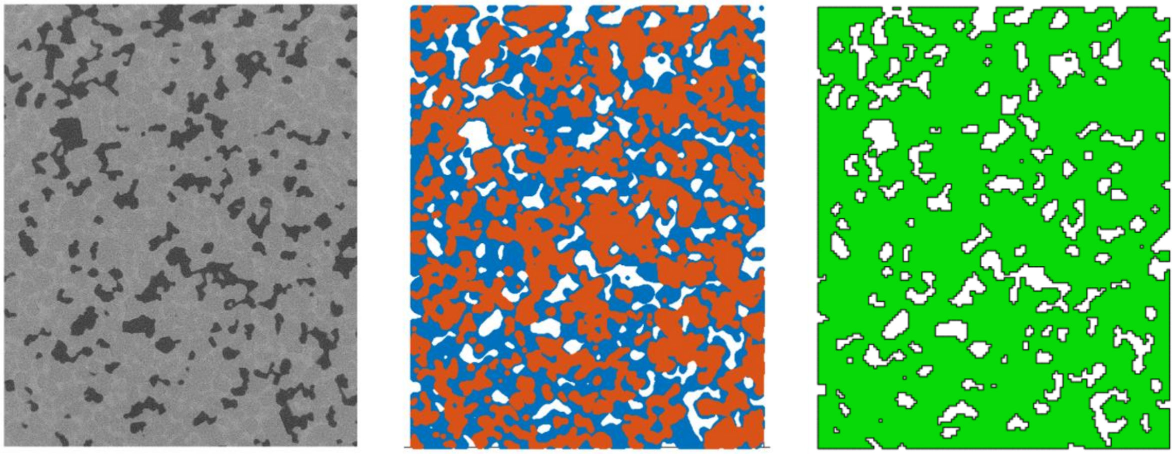

Figure 2. RVE Image, Binarized RVE, and RVE in Abaqus CAE

EXPERIMENTAL METHODS

The RVEs used in this simulation are 19 equidistant XCT image slices along the length of a sugar-PDMS compression sample that were fabricated at Virginia Tech.[3] The images are binarized to differentiate binder, voids, and grains, and this is used to generate a matrix of material flags. Each pixel from the image corresponds to a material flag in this matrix. With this matrix, a mesh can be generated in which rectangular elements each correspond to an image pixel. The meshes used in the simulation are 0.0125 m in height and 0.001 m in width. This process can be seen in Figure 2. This resultant mesh is then assigned sections and properties according to the FEA software input file format.

The software used to perform the computational compression tests was Abaqus CAE. Abaqus is a software developed by Dassault Systemes that employs Finite Element Analysis for stress, strain, heat transfer, acoustics, and several other analyses.[4] Abaqus is capable of performing both explicit and implicit simulations. For the simulations within this investigation, a standard/explicit model was used with a single timestep in which displacement is applied.

For the binder region of the RVEs, the Young’s modulus is 2.77 MPa and the Poisson’s ratio is 0.25.[5] For the sugar grains, the Young’s modulus is varied, and the Poisson’s ratio is 0.25. These material properties are assigned within the Abaqus input file to each of the elements according to the flag matrix. In addition, the element type used in Abaqus is 2D planar, deformable shell CPS4R elements (quadrilateral linear elements, plane stress, reduced integration, with hourglass control).

The simulations that were run for this experiment are compression tests, in which a 2D rectangular model is constrained in the y-direction on the bottom surface, and the top surface is displaced in the negative y-direction to cause compression. The prescribed displacement causes a strain of 6%. The left and right sides are unconstrained. This set-up can be seen in Figure 3.

With this experiment set-up, the constitutive relationship reduces to Equation 4:

$$\epsilon_{yy} = \frac{\sigma_{yy}}{E} \tag{4}$$

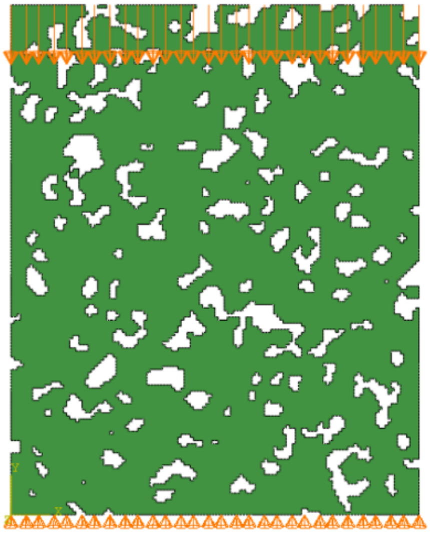

Figure 3. Example RVE with Boundary Conditions

Therefore, the effective Youngs modulus of the RVE can be determined by dividing the volume-averaged stress in the y-direction by the applied boundary strain in the y direction (6%).

Volume-averaged stress (σ_{VA}) is calculated using Equation 5 where *n* is the number of elements in the mesh and *A* is the area of an element.

$$\sigma_{VA} = \frac{\sum_{i=1}^{n}(\sigma_{yy,n} * A_n)}{\sum_{i=1}^{n}(A_n)} \qquad (5)$$

This formula applies to the full mesh area, and therefore *n* is the product of the number of elements in width and height of the mesh. The voids have a stress value of zero, but account for a finite area.

In addition, each element in the mesh has an equal area. Therefore, the volume-averaged stress formula reduces to Equation 6.

$$\sigma_{VA} = \frac{\sum_{i=1}^{n}(\sigma_{yy,n})}{n} \qquad (6)$$

In other words, the volume-averaged stress is determined by summing the σ_{yy} values for each of the elements and dividing by the notional element count if all voids were filled in by elements (this equates to the width multiplied by the height in terms of element count).

This was completed for each of the RVE's at a fixed sugar Young's modulus value, and was averaged across RVE's to find the average effective Young's modulus for a given sugar Young's modulus value.

This process was completed for a range of sugar Young's modulus values, and these data points serve as a relationship between these two variables. Therefore, the sugar Young's modulus value that results in the experimental effective Young's modulus was interpolated and simulated.

RESULTS

The first simulations that were run used a sugar Young's modulus of 120 MPa. Each RVE was run with this parameter, and the effective Young's modulus was calculated. Table 1 shows this average value with the corresponding standard deviation. Figure 4 displays the stress-strain curve for this data.

Table 1. Abaqus – Average Effective E

Sugar E (MPa)	Average E_{eff} (MPa)
120	8.1412 ± 3.22

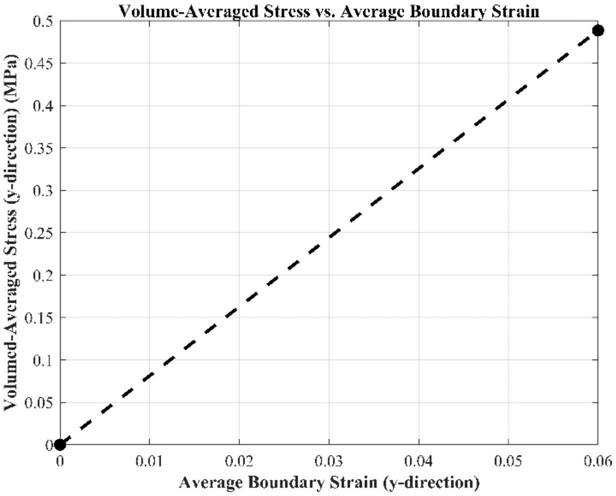

Figure 4. Stress- Strain (Sugar E = 120 MPa)

The resulting effective Young's modulus was much lower than the experimental value. Therefore, a range of values above 120 MPa was simulated.

These values serve as the points for which the experimental sugar Young's modulus can be interpolated.

A sugar Young's modulus value of 120, 240, 480, and 720 MPa was used for each set of RVEs, and the effective Young's modulus was calculated. This value was then averaged across RVEs. These values are tabulated in Table 2 and graphed in Figure 5.

Table 2. Abaqus – Average Effective E

Sugar E (MPa)	Average E_{eff} (MPa)
120	8.1412
240	10.5060
480	13.5499
720	15.7794

The standard deviation values for these E_{eff} results are 3.2197, 4.8031, 7.158, and 9.0761.

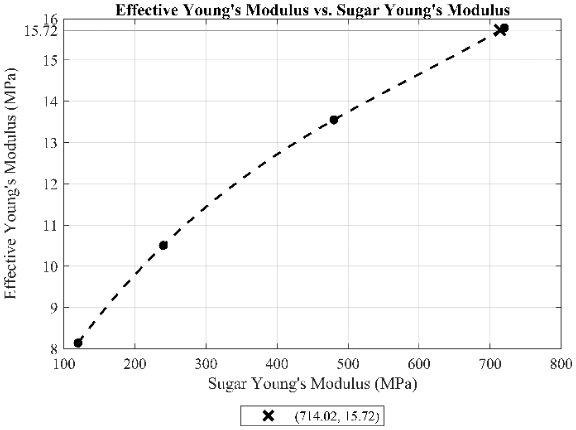

Figure 5. Effective E vs. Sugar E

With the above relationship between effective Young's modulus and sugar Young's modulus, a polynomial was used to connect the data points. A polynomial with a power of three was used. This equation revealed that an effective Young's modulus of 15.72 MPa (experimental value) will result from a sugar Young's modulus of ~714 MPa.

To confirm this interpolated value, this sugar Young's modulus was used in an Abaqus simulation. This resulted in an effective Young's modulus of 15.7294 MPa. This stress-strain plot can be seen in Figure 6.

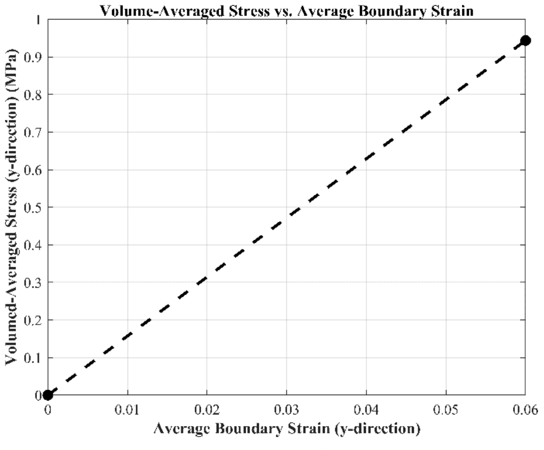

Figure 6. Stress - Strain (Sugar E = 714 MPa)

This simulation confirmed the interpolation. The output of the Abaqus simulation resulted in an effective Young's modulus of 15.7294 MPa, which is within 0.06% of the experimental value of 15.72 MPa.

CONCLUSION

For this investigation, commercial finite element analysis software (Abaqus) was used to simulate compression tests of mock energetic material. The Young's modulus of the sugar grains in the material was unknown, though the effective Young's modulus was a known value. Therefore, in order to solve this inverse problem, a range of sugar Young's modulus values was used to determine an effective RVE Young's modulus. This dataset was used to interpolate for the sugar Young's modulus that would match the effective Young's modulus which was determined experimentally. As a result, a relationship between sugar and effective Young's modulus was determined.

The sugar Young's modulus was determined to be 714.02 MPa.

This material property is a necessary component of simulating mock energetic materials. With this constituent Young's modulus, further simulations can be completed that simulate the crack propagation and damage within these materials. In addition, thermal and conductive effects can be investigated during various loading situations of mock energetic materials to further the study of damage sensing in energetic materials such as solid rocket fuel.

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