Specific Surface: A Missing Parameter in High-Explosive Modeling
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Abstract

To accurately describe the constitutive response of high explosives such as PBX 9501, we need to consider the heterogeneous explosive as a composite rather than a homogeneous solid. Because of the extremely complex nature of the structural distribution of the constituents, the phase-volume fractions alone are insufficient to characterize such a complicated microstructure. What other parameter (or parameters) do we need to consider? How do we incorporate the parameter (or parameters) into a theoretical framework for developing a constitutive theory for high explosives? In this report we identify the so-called specific surface (i.e., the interfacial area-per-unit-volume of a multi-phase heterogeneous solid) as an additional parameter used in modeling the constitutive behavior of high explosives. Both the phase-volume fractions and the specific surface are needed to characterize the microstructure of the material. This report (1) provides a detailed argument that supports this conclusion, (2) presents a method (based on optical micrographs) for estimating the specific surface of PBX 9501, and (3) discusses the characteristics of theoretical frameworks designed to construct constitutive models of high explosives.

1 Introduction

Thermal/mechanical properties may be the dominant factor in determining the safety and survivability of a high explosive during low- and moderate-strain rate, non-shock, deformation processes. Thus, developing physics-based equations of state and constitutive models presents a major challenge because such a theory would ultimately
need to address issues such as viscoelasticity, thermal effects, damage initiation and accumulation, crack formation and propagation, and chemical reactions.

Engineers use two distinct strategies to model the constitutive response of high-explosive materials. The first strategy concentrates on the average continuum properties of high explosives without regard to their origins on a micromechanical scale. The second strategy consists of modeling the high explosive as a heterogeneous composite. To develop such a model, we take into consideration the explicit behavior of the energetic crystals, the polymeric binder, and the interface between the two constituents.

One of the most important characteristics of the first strategy is that it treats the high-explosive material as a homogeneous continuum. One of the earliest models built by using this strategy is SCRAM (Statistical CRAck Mechanics, also known as SCM), which dates back 25 years (Dienes, 1978; Dienes, 1996). The SCRAM model is based on a generalized superposition of strain rates that is shown to be valid for arbitrarily large deformations. The model accounts for both opening and shear growth, as well as coalescence of cracks. Therefore, it is able to deal with the damage-induced anisotropy. Originally, every crack was assigned to one of nine different orientations, and cracks in each orientation are able to develop independently. It now appears that more than nine orientations would be required to obtain good accuracy. SCRAM also includes the chemistry for addressing burn and reaction of high explosives. A simplified version that treats crack behavior as isotropic was developed under the rubric of Isoscram.

Another variant of SCRAM, the visco-SCRAM model (Bennett et al., 1998), emphasizes the role of strain-rate effects. Visco-SCRAM treats a high explosive, such as PBX 9501, as a viscoelastic continuum that when compressed can undergo inelastic cracking. It makes no claims concerning the origin of the viscoelasticity or where the cracking occurs (matrix, inclusion, or interface). The model simply relies on empir-
ical data to calculate the modulus and peak stress as functions of strain rate and, as a result, is phenomenological in nature. Currently, the visco-SCRAM model includes effects of viscosity-induced bulk-temperature distribution (as opposed to a hot spot), inelastic cracking, chemical heating, and conduction. Implemented into several finite-element codes, this model has been used successfully to simulate several different experiments.

Models that use the second strategy include the Method of Cells (MOC) model, the three-dimensional Generalized Method of Cells (3D GMC) model, and the Dirty Binder/MOC (MOC model incorporating the dirty-binder analysis) model (Aboudi, 1991; Clements and Mas, 2000). Most of these models consider only the volume fractions of the different phases in the composite. These models have been implemented into DYNA3D and EPIC finite-element codes.

Although active efforts are continuing to develop and refine models based upon the first strategy, the past several years have seen more and more efforts directed toward the development of models that consider high explosives as composites (i.e., models based upon the second strategy). This report is intended to address issues relevant to the development of constitutive models following the second strategy.

To develop physics-based constitutive models of intrinsically heterogeneous high explosives, we must (1) understand the properties of individual constituents and (2) accurately describe the details of the microstructure. Such details include phase-volume fractions, surface areas of interfaces, orientations, sizes, shapes, spatial distribution of the phase domains, and connectivity of phases. However, to what degree we need to include the microstructural information so that we can describe the effective properties of a high explosive remains an open question awaiting both theoretical analyses and experimental measurements.

In surveying previous developments, we find that the phase-volume fractions play a key role in most of the constitutive models of composite materials. However, we
believe that the parameter of specific surface (i.e., the interfacial surface area per unit volume of a heterogeneous solid) is as important as the phase-volume fractions. A physical property, the specific surface area represents the heterogeneous nature of the high explosive. Mathematically, the information it represents is at the same level as that of the phase-volume fractions. In mathematical terms, the microstructure of a heterogeneous material can be described by an infinite set of $n$-point statistical correlation functions. Both the phase-volume fractions and the specific surface are one-point correlation functions. Our objective in this report is to extend the theoretical framework of constructing constitutive models for high explosives so that such construction incorporates both the phase-volume fractions and the specific surface in their descriptions of the material’s microstructure.

We have organized this report as follows. In Section 2, we use a simple example, uniaxial compression of the PBS 9501 sugar mock simulant material, to illustrate that we must treat high-explosive materials, such as PBX 9501, as heterogeneous composites. In Section 3, we re-examine some of the most fundamental relationships in analyzing heterogeneous solids. We will show that when the interface between different constituent phases deforms according to its own constitutive law, these fundamental relationships need to be modified and the specific surface comes into play in these modified relationships. In Section 4, we present a formal mathematical definition of the specific surface. In Section 5, we study several unit cells with inclusions of simple geometries. Such a study is important because the construction of unit cells serves as the foundation of many constitutive models. We will show that for a two-phase random composite, the variations of the specific surface can be quite large for different inclusion geometries or for a different number of inclusions in a unit cell, even when the volume fraction is held constant. In Section 6, we present a method that estimates the value of the specific surface of the PBX 9501 high explosive based on optical micrographs. The result reveals that the conventional way of constructing unit cells grossly underestimates the specific surface of PBX 9501 high explosive. Finally, in Section 7,
we discuss aspects of developing a constitutive model of high explosives that incorporates both volume fraction and specific surface. This model would not rely on the notion of a unit cell.

2 High-Explosive Materials: Homogeneous or Heterogeneous

Almost all engineering materials are heterogeneous in nature. They are either compounds of several different phases or aggregates of crystals with different sizes and orientations. Damage and failure mechanisms are also inhomogeneous. We may treat these materials as either homogeneous or heterogeneous, depending on the length scale of the problem we are addressing.

One popular opinion, which we take for granted, is that a material can be treated as homogeneous or uniform if the characteristic length of the process under consideration is many magnitudes larger than the material’s microscopic length scale. The advantage of assuming the material is homogeneous is that many well-developed theories are available for describing its constitutive behavior. Moreover, the mathematical treatment of homogeneous materials is straightforward. However, high explosives cannot be treated as homogeneous, even though their average crystal size is very small and the volume fraction of the second phase (polymeric binder) is less than 5%. This is because damage, or microcracking, is the most important deformation mechanism in high explosives, and the formation of microcracks cannot be explained satisfactorily on the basis of homogeneous assumptions.

Liu et al. (2001) have estimated the driving force that triggers the initiation of damage for the uniaxial compression of PBS 9501 sugar mock. This estimate is based on a theory that explicitly treats the high explosive as a heterogeneous composite. We will summarize their findings in the paragraphs that follow.

For this experimental investigation we used the high-explosive simulant material PBS 9501. Although inert, PBS 9501 simulates, at the macroscopic level, the mechani-
cal behavior of PBX 9501 as a function of strain rate and temperature. Both PBX 9501 and PBS 9501 consist of very high volume fractions of crystalline phase bonded with a polymeric binder. PBS 9501 consists of 94 wt% C&H granulated sugar, whereas the actual high explosive has 95 wt% crystalline HMX energetic crystals. The sugar and HMX crystals are monoclinic and microscopically similar. Both PBS 9501 and PBX 9501 have the same polymeric binder system, which consists of 50% estane and 50% nitroplasticizer.

When a heterogeneous material is subjected to homogeneous boundary conditions, the deformation field below a certain length scale becomes non-uniform. Hence, to investigate the heterogeneity and heterogeneity-induced damage, we needed a technique that could monitor the full-field deformation throughout the entire sample.

We developed an optical technique called dot-matrix deposition and mapping. In principle, this technique is very similar to the image correlation method (Chu et al., 1985), but it avoids the ambiguity regarding the reflectivity of the specimen surface during the deformation process. The specimen reflectivity will change as damage occurs. Before experiment, we deposit a matrix of dots on the surface of the specimen. We then photograph the pattern at different moments during deformation.

One such photograph is shown in Fig. 1(a). This image is then processed to identify the exact location of the center of each dot. Based on the coordinates of each dot, an element mesh, as shown in Fig. 1(b), is constructed for the moments before and after deformation. By assuming that each element is undergoing homogeneous deformation, we can calculate all three in-plane strain components of each element by using the coordinates of its four nodes. Figure 1(c) shows the field plot for each strain component, which corresponds to the deformed state shown in Fig. 1(b). The formulation for obtaining the strain components of each element is valid for finite deformation, including the locally large deformation associated with damage.

Figure 2 shows the lateral strain component $\epsilon_{11}$, at two moments, A and B, during
Figure 1: (a) Dot-matrix image during deformation; (b) element meshes before and after deformation; and (c) field plots of all three in-plane strain components corresponding to the deformed state.

In Fig. 3, we consider two consecutive moments along the loading curve. At time C, the compressive load is 360 N and by time D, the compressive load has increased the early stage of loading. The scatter plot illustrates the strain magnitude of each element and the distribution plot shows the percentage of elements that experience certain strain. If the material were homogeneous, every element would deform exactly the same amount at the same time. In such a case, all data points in the scatter plot would fall onto a single horizontal line, whereas in the distribution plot the data points would form a vertical line. The deformation of each element shown in Fig. 2 scatters around a mean value. In the early loading stage, the distribution plot maintains one shape; the only shift is the mean value, which corresponds to the deformation of the entire specimen. The shape of strain distribution reflects the heterogeneous nature of the material. Note that the size of a dot-matrix element is approximately $1 \text{ mm} \times 1 \text{ mm}$. On average, approximately several hundred PBS sugar crystals fit in this element.
Figure 2: Strain distribution showing heterogeneous deformation during the early loading stage.

to 432 N. During this small increment of loading, the distribution shape of the lateral strain component, $\epsilon_{11}$, changes drastically. The change signals the initiation of damage within the test specimen. At time C, the shape of the distribution of $\epsilon_{11}$ is unchanged from times A and B. By time D, several elements are at a much larger strain: two at tensile strain and two at compressive strain. Simple analysis shows that the cracking of a material element under compression causes an additional strain increment in the lateral direction. Therefore, the two elements that exhibit larger tensile strain must also experience cracking. At time D, when damage initiates, the compressive stress is only 44% of the material’s compressive strength. We must point out that the two elements with larger compressive strains are adjacent to those at a large tensile strain. When internal cracking occurs in an element, the element expands more in the lateral direction. As a result, the neighboring element compresses to keep the overall deformation compatible.

At time D, if we ignore the four elements at larger strains, we find a distribution of the strain component $\epsilon_{11}$ similar to that at previous moments. This suggests that the
damage is confined to the four individual elements. On the other hand, if the damage extends over many elements, we would have seen a change in the overall shape of the strain distributions. This situation exists at times E and F, as shown in Fig. 4. The broadness of the strain distribution thus provides a means for monitoring damage evolution in the specimen.

Figure 3: Indication of damage initiation in the specimen under compression.

Figure 4: Indication of damage accumulation and evolution in a specimen under compression.

Investigators have conducted many theoretical studies to explain the appearance of splitting cracks during the compression in brittle solids. In one such investigation,
Nemat-Nasser and Horii (1982) proposed a theory that requires pre-existing cracks within the sample. Although most brittle materials contain processing microcracks before loading, an accurate description of the distribution of these cracks proves to be very difficult, if not impossible. Meanwhile, most micromechanical analyses treat the matrix material as homogeneous. From the experimental strain distributions shown in Fig. 2, we see that the material exhibits heterogeneity prior to the initiation of damage. To study the initiation of damage in compression, it would be more appropriate to apply a theory that treats the simulant material as a heterogeneous composite.

Ortiz (1985) proposed a general framework for the constitutive modeling of concrete. He started from the first principles of mechanics based on the theory of interacting continua or mixture theory and included a rate-independent theory of damage. An important feature of this framework is that the concrete is treated explicitly as a mixture of two distinct phases: mortar and aggregate. Because of this assumption, Ortiz found that the externally applied stresses distribute unequally between the two phases. The average stresses acting in mortar and aggregate must jointly equilibrate the applied loads but may be vastly different from each other. In the paragraphs that follow, we will adopt a very simple version of this mixture theory to demonstrate that a purely compressive uniaxial load will induce tensile stresses normal to the loading axis within the crystal. These tensile stresses are high enough to initiate damage before the overall compressive load reaches its peak value.

Consider a material element in which the volumetric fractions of the crystal and the binder are \( f_1 \) and \( f_2 \), respectively. Let \( \sigma_1 \) and \( \sigma_2 \) be the average or phase stresses acting in crystal and binder, whereas \( \sigma \) will represent the applied stress. The requirement that \( \sigma_1 \) and \( \sigma_2 \) jointly equilibrate \( \sigma \) can be expressed as

\[
\sigma = f_1 \sigma_1 + f_2 \sigma_2. \tag{2.1}
\]

If we consider a “virgin” high-explosive specimen and assume that both crystal and binder are isotropic and elastic, the phase stresses \( \sigma_1 \) and \( \sigma_2 \) can be related to the
applied stress $\sigma$ through

$$(\sigma_a)_{ij} = \frac{1}{3} \left( \frac{k_\alpha}{k} - \frac{\mu_\alpha}{\mu} \right) \sigma_m \delta_{ij} + \frac{\mu_\alpha}{\mu} \sigma_{ij}, \quad \alpha = 1, 2,$$

(2.2)

where $k_\alpha$ and $\mu_\alpha$ are the bulk and shear moduli of each constituent and $k$ and $\mu$ are the bulk and shear moduli for the composite. Under uniaxial compression, where external stress is characterized by $\sigma_{ij} = -\sigma \delta_{i1} \delta_{j1}$ and $\sigma > 0$ is the magnitude of the applied compressive stress, the phase stress within crystal $\sigma_1$ has the following form:

$$(\sigma_1)_{ij} = \begin{bmatrix} \sigma_L & 0 & 0 \\ 0 & \sigma_T & 0 \\ 0 & 0 & \sigma_T \end{bmatrix}, \quad \sigma_L = -\frac{1}{3} \left( \frac{k_1}{k} + \frac{2\mu_1}{\mu} \right) \sigma, \quad \sigma_T = \frac{1}{3} \left( \frac{\mu_1}{\mu} - \frac{k_1}{k} \right) \sigma.$$

(2.3)

Experimental measurements have shown that the binder material is almost incompressible (i.e., its Poisson’s ratio $\nu_2 \simeq 0.5$). One can show that

$$\frac{\sigma_T}{\sigma} = \frac{1}{3f_1} \left\{ 1 + \frac{2(1 + \nu_1)}{3} \cdot \frac{f_2E_2}{f_1E_1} \right\}^{-1},$$

(2.4)

where $\nu_1$ is the Poisson’s ratio of the crystal and $E_1$ and $E_2$ are the Young’s moduli of the crystal and the binder, respectively. PBS 9501 yields the following: $f_1 \simeq 0.96$ and the Poisson’s ratio of the crystal $\nu_1 \simeq 0.2$. Within a wide strain-rate regime, the ratio of $E_2/E_1$ is on the order of $10^{-3}$. As a result, the second term in the braces of the above expression is negligible. This fact leads to $\sigma_T/\sigma \simeq 1/3f_1 = 0.35$. We can also show that the lateral stress within the binder is almost zero.

Figure 5 shows a typical uniaxial compression test of PBS 9501. The solid line in the figure shows the apparent stress-strain curve. The applied uniaxial stress is a monotonically increasing function of the axial strain until it reaches the maximum value. After this point, stress decreases gradually as the deformation continues to proceed. If we take a crystal element from the compressive sample, we can characterize the phase stress within the crystal by $\sigma_L$, which is compressive and parallel to the externally applied load, and by $\sigma_T$, which is tensile and normal to the loading axis. The variation of the lateral tensile stress $\sigma_T$ is shown as dash-dotted line in Fig. 5. Experimental measurement also showed that the tensile strength of PBS 9501 material is only
approximately 15% of its compressive strength. If we assume that in tension failure is mainly caused by crystal cracking, we can conclude that microcracks start to develop in crystals when \( \sigma_T \approx 0.15 \sigma_C \). The onset strain for microcrack initiation within the compressive sample is indicated by the vertical dash-line shown in Fig. 5. Therefore, damage initiation occurs when the compressive stress \( \sigma \approx 0.42 \sigma_C \). This prediction matches the experimental observation shown in Fig. 3.

Immediately after damage initiation, there are so few microcracks within the sample that they do not interact with each other. The enlargement of such cracks remains a stable process because of the stress redistribution between the crystal and the binder. The applied stress keeps increasing as deformation continues. However, unstable crack propagation begins when the size or the density of microcracks becomes large enough that the stress redistribution cannot ensure stable crack growth. This unstable cracking is responsible for generating the characteristic descending branch of the uniaxial compressive stress-strain curve shown in Fig. 5.

Liu et al. (2001) proved that damage in high-explosive materials is the direct consequence of heterogeneity, which is manifested by the significant mismatch of the elastic constants between the energetic crystal and the polymeric binder. Because the mixture
theory explicitly treats the material as a heterogeneous composite, we can correctly predict failure in a uniaxial compression sample without resorting to any artificial mechanisms.

Treating high-explosive material as a heterogeneous composite suggests that its constitutive behavior results from three concurring factors: the elastic behavior of the energetic crystal, the constitutive response of the polymeric binder, and the interaction between the crystal and the binder (i.e., the behavior of the interface). However, in the framework proposed by Ortiz (1985), the only quantity that characterizes the material’s composition is the volume fraction of each constituent. The behavior of the interface between the different phases is not accounted for in Ortiz’s theory.

Another methodology popular in the modeling of composite behavior is based on the notion of unit cells. A simple cell is constructed based upon some of the material’s microstructural information. We then conduct detailed continuum-mechanics analysis on this simple cell to establish the relationship between the applied load and the overall response of the cell. This methodology is applicable to general loading conditions, compatible with a variety of constitutive relations for the constituent materials and interfaces, and easy to implement as the material model in existing continuum analysis. However, high-explosive materials present some extremely difficult issues that challenge the unit-cell methodology. For example, the microstructure of high-explosive materials is very random and chaotic, with severe variations in both the inclusion sizes and orientations, as well as complicated damage formation and accumulation mechanisms. It is very difficult, if not impossible, to construct a simple unit cell capable of representing the random and chaotic microstructure of high-explosive materials.

In the following sections, we will show that both the phase-volume fractions and the specific surface (i.e., the interfacial area between phases per unit volume) play equally important roles in characterizing the composition of a heterogeneous mate-
rial. We will also show that simple representative volume elements, often used in the analyses, typically cannot capture both the phase-volume fractions and the specific surface. Indeed they usually grossly underestimate the amount of interface within a material element.

3 Fundamental Relations in Mechanics of Heterogeneous Solids

In studying the macroscopic stress-strain relations of a heterogeneous solid, where the macroscopic or overall response of the material is still homogeneous, a block of the material called representative volume element (RVE) is often considered. Through micromechanics analysis, the macroscopic stress and strain of the element are related to the microscopic stress and strain, which by definition are nonuniform within the volume. The macroscopic stress-strain relation for the heterogeneous material is then established as a function of the properties of the different phases within the element.

Key to the micromechanics analysis is the evaluation of the macroscopic (or average) strain and stress of the volume element. There are two methods to calculate the macroscopic strain and stress from their microscopic counterparts. One is the straightforward volume average (Hill, 1963) so that the macroscopic value of a quantity is its integral over a specified region divided by the volume of the region. The other way of calculating the average is through the work conjugate (Rice, 1970). For example, the average strain is the work conjugate of the prescribed average stress, in terms of the prescribed uniform surface traction on the outer surface of the volume element. Rice (1970) also pointed out that the averages calculated by both schemes are equivalent.

However, this conclusion is valid only when the interface between different phases makes no contribution to the overall mechanical response of the material element. The purpose of this section is to examine the differences between the abovementioned averaging schemes when the interface between different phases is allowed to behave according to its own constitutive rule. For sake of simplicity, we only consider a two-
phase composite in this section, but the conclusion can be easily extended to multi-phase heterogeneous materials.

3.1 Average of strain

Consider a material element \( R \) of a two-phase composite, where the volume of the element is \( V \). The element \( R \) is the union of two disjoint subelements \( R_1 \) and \( R_2 \), or \( R = R_1 \cup R_2 \) and \( R_1 \cap R_2 = \emptyset \), with volumes \( V_1 = f_1 V \) and \( V_2 = f_2 V \), respectively, where \( f_1 \) and \( f_2 \) are the phase-volume fractions and \( f_1 + f_2 = 1 \). The element has an interfacial area between the two phases of \( S_{\text{int}} = s V \), where \( s \) is the specific surface of the composite. We assume that the microstructure within this material element is random and that the spatial distribution of the different phases is such that the response of the composite material is homogeneous, so long as the material elements are large enough (larger than the so-called minimum RVE).

This sample element is then subjected to a homogeneous macroscopic stress state \( \Sigma \). More precisely, such a state is realized through the application of a surface traction \( t \) on the outer boundary of the element, \( \partial R \), by

\[
t_i = \Sigma_{ij} n_j,
\]

where \( n \) is the outward unit normal of \( \partial R \). Associated with this homogeneous macroscopic stress \( \Sigma \), the sample element will deform and that will lead to a certain amount of displacement on the surface of the element. The macroscopic strain \( E \) associated with any set of surface displacements \( u \) is defined by requiring that \( E_{ij}\Sigma_{ij} \) be the specific work in carrying tractions corresponding to any stress state \( \Sigma \) through those displacements:

\[
(S_{\text{ij}}E_{ij})V = \int_{\partial R} (\Sigma_{ij}n_j)u_i \, dA.
\]

Validity for any \( \Sigma \) and symmetry of the strain tensor then implies that

\[
E_{ij} = \frac{1}{V} \int_{\partial R} \frac{1}{2}(u_i n_j + u_j n_i) \, dA.
\]
This definition was given by Rice (1970).

According to the volume-average scheme (Hill, 1963), the average strain of the sample element, denoted by $E^*$ to differentiate it from that in equation (3.3), can be calculated through

$$E^*_{ij} = \frac{1}{V} \int_V \varepsilon_{ij} \, dV,$$  

(3.4)

where $\varepsilon$ is the local strain within the sample element and therefore, is nonuniform. Moreover, we can write

$$\frac{1}{V} \int_V \varepsilon_{ij} \, dV = \frac{1}{V} \left( \int_{V_1} \varepsilon_{ij} \, dV + \int_{V_2} \varepsilon_{ij} \, dV \right),$$

for the two-phase composite. Furthermore,

$$\int_{V_a} \varepsilon_{ij} \, dV = \int_{\partial V_a} \frac{1}{2} (u_{ij} + u_{ji}) \, dA = \int_{\partial V_a} \frac{1}{2} (u_{i,n} + u_{j,n}) \, dA, \quad \alpha = 1, 2. \quad (3.5)$$

Note that $\partial V_a = S^{(\alpha)}_{\text{out}} + S_{\text{int}}$, where $S^{(\alpha)}_{\text{out}}$ is part of the outside surface of material element $R$ that comes from phase $\alpha$. As a result, we have

$$\int_{V} \varepsilon_{ij} \, dV = \int_{\partial R} \frac{1}{2} (u_{i,n} + u_{j,n}) \, dA$$

$$+ \int_{S_{\text{int}}} \frac{1}{2} (u^{(1)}_{i,n} + u^{(1)}_{j,n}) \, dA + \int_{S_{\text{int}}} \frac{1}{2} (u^{(2)}_{i,n} + u^{(2)}_{j,n}) \, dA. \quad (3.6)$$

Along the interface $S_{\text{int}}$, we define $u^{(1)}_{i} = u^{-}_{i}$, $u^{(2)}_{i} = u^{+}_{i}$, and $n^{(1)}_{i} = -n^{(2)}_{i} = n_{i}$ so that the normal $n_{i}$ is pointing from the $(-)$ side to the $(+)$ side. Now, equation (3.4) becomes

$$E^*_{ij} = \frac{1}{V} \int_{\partial R} \frac{1}{2} (u_{i,n} + u_{j,n}) \, dA - \frac{1}{V} \int_{S_{\text{int}}} \frac{1}{2} ([u_{i}]n_{j} + [u_{j}]n_{i}) \, dA,$$  

(3.7)

where $[u_{i}] = u^{+}_{i} - u^{-}_{i}$ ($i = 1, 2, 3$) is the displacement jump across the interface.

By comparing equations (3.3) and (3.7), one has

$$E_{ij} = E^*_{ij} + s E^\text{int}_{ij},$$  

(3.8)

where

$$E^\text{int}_{ij} = \frac{1}{S_{\text{int}}} \int_{S_{\text{int}}} \frac{1}{2} ([u_{i}]n_{j} + [u_{j}]n_{i}) \, dA,$$
and \( s = \frac{S_{\text{int}}}{V} \) is the specific surface of the material element. Equation (3.8) establishes the relationship between the two average strains. Also note that when the bonding between the two phases is perfect (i.e., \([ u_i ] = 0\) for \( i = 1, 2, 3 \) on \( S_{\text{int}} \)), the two average strains become identical.

### 3.2 Average of stress

Now let the sample element be subjected to a homogeneous macroscopic strain \( E \) by applying a displacement field \( u \) on the outer surface of the element, where

\[
u_i = E_{ij} x_j, \quad \forall x_i \in \partial R.
\]

By the same work conjugate argument, the macroscopic (or average) stress \( \Sigma \) is given by

\[
\Sigma_{ij} = \frac{1}{V} \int_{\partial R} \frac{1}{2} (t_i x_j + t_j x_i) \, dA,
\]

where \( t \) is the surface traction due to the applied boundary displacement.

On the other hand, one can calculate the macroscopic stress \( \Sigma^* \) through the volume average,

\[
\Sigma^*_{ij} = \frac{1}{V} \int_V \sigma_{ij} \, dV,
\]

where \( \sigma \) is the local stress within the element and is nonuniform. Furthermore, one can show that

\[
\int_V \sigma_{ij} \, dV = \int_V \sigma_{ik} \delta_{jk} \, dV = \int_V \sigma_{jk} x_{ik} \, dV = \int_V (\sigma_{ik} x_j)_{ik} \, dV
\]

\[
= \int_{V_1} (\sigma_{ik} x_j)_{ik} \, dV + \int_{V_2} (\sigma_{ik} x_j)_{ik} \, dV = \int_{\partial R_1} (\sigma_{ik} n_k) x_j \, dA + \int_{\partial R_2} (\sigma_{ik} n_k) x_j \, dA
\]

\[
= \int_{\partial R} t_i x_j \, dA + \int_{S_{\text{int}}} t_i^{(1)} x_j \, dA + \int_{S_{\text{int}}} t_i^{(2)} x_j \, dA = \int_{\partial R} t_i x_j \, dA,
\]

with the help of the equilibrium equation and the divergence theorem, and by noting the fact that \( t^{(1)} = -t^{(2)} \) along the interface. As a result of the symmetry of the stress tensor \( \sigma \), we have

\[
\Sigma^*_{ij} = \frac{1}{V} \int_{\partial R} \frac{1}{2} (t_i x_j + t_j x_i) \, dA.
\]
This is exactly the same as that given in equation (3.10). Therefore, the two averaging schemes yield the same macroscopic stress of the material element.

### 3.3 The basic lemma

A basic lemma (Hill, 1967) has been used frequently to determine the effective or homogenized behavior of heterogeneous composites (e.g., see Ponte Castañeda and Suquet, 1998). Because of its importance, we restate it in the following: Consider the material element \( R \) with volume \( V \). Let \( \sigma \) be a divergence-free stress field and \( u \) a displacement field, and they satisfy the traction boundary condition,

\[
\sigma_{ij} n_j = \Sigma_{ij} n_j, \quad \forall \; x_i \in \partial R, \tag{3.13a}
\]

and the displacement boundary condition,

\[
u_i = E_{ij} x_j, \quad \forall \; x_i \in \partial R, \tag{3.13b}
\]

respectively. Then there is

\[
\Sigma_{ij} E_{ij} = \frac{1}{V} \int_V \sigma_{ij} \varepsilon_{ij} \, dV, \tag{3.14}
\]

where \( \varepsilon_{ij} = (u_{ij,j} + u_{ji,i})/2 \). Note that in equation (3.14), \( \sigma \) and \( \varepsilon \), as well as \( \Sigma \) and \( E \), are not necessarily related by a constitutive relation.

Once again, relation (3.14) is only valid when the effects from interface between different phases are neglected. When the interface is also allowed to deform, the volume integration in the right-hand side of equation (3.14) can be written as

\[
\int_V \sigma_{ij} \varepsilon_{ij} \, dV = \int_V \sigma_{ij} u_{ij,j} \, dV = \int_V (\sigma_{ij} u_i)_j \, dV
\]

\[
= \int_{V_1} (\sigma_{ij} u_i)_j \, dV + \int_{V_2} (\sigma_{ij} u_i)_j \, dV = \int_{\partial V_1} \sigma_{ij} n_j u_i \, dA + \int_{\partial V_2} \sigma_{ij} n_j u_i \, dA.
\]

Again, note that \( \partial V_\alpha = S_{\text{out}}^{(\alpha)} + S_{\text{int}} \), where \( S_{\text{out}}^{(\alpha)} \) is part of the outside surface of material element \( R \) that comes from phase \( \alpha \), and \( S_{\text{int}} \) is the interface between different phases,
we have
\[ \int_V \sigma_{ij} \epsilon_{ij} \, dV = \int_{\partial R} t_i u_i \, dA + \int_{S_{\text{int}}} t_i^{(1)} u_i^{(1)} \, dA + \int_{S_{\text{int}}} t_i^{(2)} u_i^{(2)} \, dA. \] (3.15)

The first term in the right-hand side of equation (3.15) can be related to the macroscopic stress and strain by imposing the boundary conditions (3.13),
\[ \int_{\partial R} t_i u_i \, dA = \int_{\partial R} \Sigma_{ij} n_j E_{ik} x_k \, dA = \Sigma_{ij} E_{ik} \int_{\partial R} x_k n_j \, dA = \Sigma_{ij} E_{ik} \int_{V} x_k n_j \, dV = \left( \Sigma_{ij} E_{ij} \delta_{ij} \right) V = \left( \Sigma_{ij} E_{ij} \right) V. \]

Finally, using the convention introduced in Section 3.1, we can show that the basic lemma in equation (3.14) becomes
\[ \Sigma_{ij} E_{ij} = \frac{1}{V} \int_V \sigma_{ij} \epsilon_{ij} \, dV + s \left\{ \frac{1}{2S_{\text{int}}} \int_{S_{\text{int}}} \sigma_{ij} \left( u_i \right) n_j + \left( u_j \right) n_i \, dA \right\}. \] (3.16)

where, once again, \( \left[ u_i \right] (i = 1, 2, 3) \) is the displacement jump across interface and \( s \) is the specific surface. Also, we need to emphasize again that \( \sigma \) and \( \epsilon \), as well as \( \Sigma \) and \( E \), are not necessarily related by a constitutive relation. One can observe that equations (3.14) and (3.16) become identical under one of two conditions: (1) either the interface is traction-free (i.e., \( \sigma_{ij} n_j = 0 \) for \( i = 1, 2, 3 \)) like cracks or voids (2) or the bonding of the interface is perfect (i.e., \( \left[ u_i \right] = 0 \) for \( i = 1, 2, 3 \)).

In this section, we re-examined some fundamental relations in mechanics of heterogeneous solids. In particular, we investigated ways of calculating the macroscopic strain and stress when taking into account the contributions from the constitutive response of the interface between different phases. We found that the two averaging schemes will lead to different macroscopic strains, whereas the resultant macroscopic stresses remain the same. The macroscopic strains from the two averaging schemes are related by a simple relationship that depends on the average deformation of the interface and the amount of interface area within the element via the specific-surface parameter. We also modified the basic lemma in mechanics of heterogeneous solids to include the effect of the interface. Again, the modified basic lemma depends on the
parameter of specific surface. To obtain the constitutive relation of the heterogeneous material, we need to establish a connection between the macroscopic strain \( E \) and the macroscopic stress \( \Sigma \). Therefore, both phase-volume fractions and specific surface will play important roles in the construction of the constitutive model for the composite.

4 Specific Surface: Definition

In the preceding section, we found that the parameter of specific surface, \( s \), becomes an important factor in describing the constitutive response of a heterogeneous solid when the interface between different phases is allowed to deform according to its own constitutive law. Parameter \( s \) signifies the amount of contribution from the interface to the overall response of a heterogeneous material element. In this section, we introduce a formal definition of specific surface, \( s \), and describe the relationship of the parameter to other correlation functions that characterize the microstructure of a random composite.

Again, consider a two-phase random composite that occupies a region \( \mathbb{R} \) in Euclidean space with a volume of \( V \). The region \( \mathbb{R} \) is the union of two disjoint subregions \( \mathbb{R}_\alpha (\alpha = 1, 2) \). In other words, \( \mathbb{R} = \mathbb{R}_1 \cup \mathbb{R}_2 \) and \( \mathbb{R}_1 \cap \mathbb{R}_2 = \emptyset \). Each subregion \( \mathbb{R}_\alpha \) consists of a phase \( \alpha \), with volume \( V_\alpha \), and volume fraction \( f_\alpha = V_\alpha / V \). For a given microstructure of the region, we may define the characteristic function of phase \( \alpha = 1 \), \( \phi_1(x) \), by

\[
\phi_1(x) = \begin{cases} 
1, & \text{for } x \in \mathbb{R}_1, \\
0, & \text{for } x \in \mathbb{R}_2.
\end{cases}
\]  

(4.1)

The characteristic function for the interface, \( \omega(x) \), is defined as

\[
\omega(x) = |\nabla \phi_1(x)|, \quad \text{for } x \in \mathbb{R}.
\]  

(4.2)

Note that \( \omega(x) \) is a generalized function, which is non-zero only when \( x \) is on the interface.
The simplest morphological measures of a medium’s microstructure are the one-point correlation functions. Among them are the phase-volume fractions $f_{\alpha} (\alpha = 1, 2)$ and the specific surface, $s$, which is defined as the interfacial surface area per unit volume of a heterogeneous solid. These two morphological quantities can be calculated through the characteristic functions $\phi_1(x)$ and $\omega(x)$ through

$$ f_1 = \langle \phi_1(x) \rangle \equiv \frac{1}{V} \int_{\mathbb{R}} \phi_1(x) \, dV, \quad s = \langle \omega(x) \rangle \equiv \frac{1}{V} \int_{\mathbb{R}} \omega(x) \, dV. \quad (4.3) $$

Obviously, $f_2 = 1 - f_1$. The first equation in (4.3) is quite trivial, but the second one is not. Without going through a formal mathematical proof, we will use a simple example to illustrate the relations in equation (4.3).

Consider a cubic unit cell of a two-phase heterogeneous material, as shown in Fig. 6. The figure shows that at the center of the unit cell there is a spherical inclusion of phase 1. The radius of the inclusion is $r_1$. The region outside the inclusion is occupied by phase 2. In the spherical coordinate system $(r, \psi, \theta)$ with the origin located at the center of the spherical inclusion, the two characteristic functions, $\phi_1(x)$ and $\omega(x)$, can be written as

$$\phi_1(x) = \phi_1(r, \psi, \theta) = \begin{cases} 
1, & \text{for } 0 \leq r \leq r_1, \ 0 \leq \psi \leq 2\pi, \ 0 \leq \theta \leq \pi, \\
0, & \text{for } r > r_1, \ 0 \leq \psi \leq 2\pi, \ 0 \leq \theta \leq \pi,
\end{cases}$$

Figure 6: A simple unit cell of a two-phase heterogeneous material.
and
\[
\omega(x) = \omega(r, \psi, \theta) = \delta(r - r_1), \quad \text{for} \quad r \geq 0, \ 0 \leq \psi \leq 2\pi, \ 0 \leq \theta \leq \pi.
\]
Now, by substituting the above two expressions into equation (4.3), we have
\[
\langle \phi_1(x) \rangle = \frac{1}{V} \int_R \phi_1(x) \, dV = \frac{1}{V} \int_0^{r_1} \int_0^{2\pi} \int_0^\pi r^2 \sin \theta \, dr \, d\psi \, d\theta \\
= \frac{1}{V} \int_0^{r_1} r^2 \, dr \int_0^{2\pi} \sin \theta \, d\theta = \frac{1}{V} \left( \frac{4}{3} \pi r_1^3 \right) = \frac{V_1}{V} \equiv f_1,
\]
and
\[
\langle \omega(x) \rangle = \frac{1}{V} \int_R \omega(x) \, dV = \frac{1}{V} \int_{r_1 - \epsilon}^{r_1 + \epsilon} \int_0^{2\pi} \int_0^\pi \delta(r - r_1) r^2 \sin \theta \, dr \, d\psi \, d\theta \\
= \frac{1}{V} \left( r_1^2 \int_0^{2\pi} \sin \theta \, d\theta \int_0^\pi \sin \theta \, d\theta \right) = \frac{4\pi r_1^2}{V} = \frac{A}{V} \equiv s.
\]
In the above, \( \epsilon > 0 \) is an arbitrary small number such that the spherical surface \( r = r_1 + \epsilon \) is still within the region of the cube and \( A \) is the surface area of the spherical inclusion.

The phase-volume fraction \( f_\alpha \) has a simple probabilistic interpretation in that it is the probability of finding a point \( x \) in phase \( \alpha \). Both phase-volume fractions, \( f_\alpha \), and specific surface, \( s \), are one-point correlation functions simply because, as shown in equation (4.3), they only involve the evaluation of the characteristic functions one point at a time in the region.

The specific surface \( s \) can also be calculated through the so-called two-point correlation function. For a two-phase heterogeneous solid, which is macroscopically isotropic, the two-point correlation function \( p_2(r) \) is defined by
\[
p_2(r) = \langle \phi_1(x) \phi_1(x + \delta x) \rangle, \quad (4.4)
\]
where \( r = \sqrt{(\delta x) \cdot (\delta x)} \) and \( \phi_1(x) \) is the characteristic function of phase \( \alpha = 1 \), which was defined previously. The probabilistic interpretation of the two-point correlation function \( p_2(r) \) is that it is the probability that two points separated by a fixed distance
$r$ both lie in phase $\alpha = 1$. The two-point correlation function $p_2(r)$ has some important properties and they are (Torquato, 2002) that

$$p_2(0) = f_1, \quad \lim_{r \to \infty} p_2(r) = f_1^2, \quad (4.5)$$

and

$$\left. \frac{dp_2(r)}{dr} \right|_{r=0} = -\frac{s}{a}, \quad (4.6)$$

where $a$ is a parameter depending on the number of dimensionality of the region being considered, $a = 2$ for one-dimensional regions, $a = \pi$ for two-dimensional regions, and $a = 4$ for three-dimensional regions, respectively. Note that both $f_1$ and $s$ characterize the behavior of the two-point correlation function $p_2(r)$ at $r = 0$.

To date most composite theories only consider the phase-volume fraction as the characterizing parameter of the composition of a composite. These theories either neglect the interface at the very onset, or they treat the interface as a secondary parameter (i.e., construct a model such that the phase-volume fraction is consistent with the composition of the composite, whereas the amount of interface area is whatever the model turns out). In Section 5, we will show that different unit cells result in a very different amount of interface area between the different phases, even when the volume fraction is kept constant.

## 5 Specific Surface of a Unit Cell with Inclusions of Simple Geometry

We can determine with a degree of certainty the specific surface of a given composite, so long as (1) we know the phase-volume fractions accurately and (2) the shape and size of the inclusions have been well characterized. As a result, we can consider specific surface as a secondary parameter, one that depends on phase-volume fractions and other known microstructural information of the material. In reality, however, the microstructure of PBX 9501, as well as any other explosive, is very complicated. For example, the distributions of both the shapes and the sizes of the energetic crystal
cover a very wide range. In this section, we will use a simple example to argue that we might be better off to treat both the phase-volume fractions and the specific surface as independent parameters.

Consider a two-dimensional unit cell of a two-phase heterogeneous solid, with the shape of a square and the size of $L_0$ (see Fig. 7). We assume an inclusion described by a regular polygon. Each edge of the polygon-shaped inclusion has the length $a$ with an angle between edges $2\pi - \theta$, where $\theta = 2\pi / n$ and $n$ is the number of edges of the polygon. The area of the regular polygon $A$ is given by

$$A = \frac{na^2}{4} \left( \tan \frac{\pi}{n} \right)^{-1}. \tag{5.1}$$

If the volume fraction of the inclusion phase is $f$ (i.e., $f = A/L_0^2$), then the length of each edge of the polygon $a$ can be written in terms of the volume fraction $f$ and the number of edges $n$ as

$$a = L_0 \sqrt{\frac{4f}{n}} \tan \frac{\pi}{n}. \tag{5.2}$$

For this two-dimensional case, the specific surface, $s$, is given by $s = na/L_0^2$. We can also rewrite $s$ in a non-dimensional fashion:

$$L_0s = 2\sqrt{\pi f} \sqrt{\frac{n}{\pi}} \tan \frac{\pi}{n}. \tag{5.3}$$

Note that as the number of edges becomes very large, $n \to \infty$, the inclusion becomes a circle, and $(n/\pi) \tan(\pi/n) = 1$. Unlike the volume fraction, which is independent of
any length scale, the specific surface \( s \) of the unit cell (as shown in Fig. 7) does depend on the size of the unit cell.

Figure 8(a) shows the variation of the normalized specific surface, \( L_0 s / 2 \sqrt{\pi f} \), as a function of the number of edges of the regular polygon-shaped inclusion. We assumed that there is only one inclusion in the unit cell and we normalized the specific surface \( s \) so that it equals to one for a given phase-volume fraction \( f \) when the shape of the inclusion becomes a circle. For a digon, or \( n = 2 \), the normalized specific surface approaches infinity. For a triangular inclusion, or \( n = 3 \), \( L_0 s / 2 \sqrt{\pi f} = 3^{3/4} / \sqrt{\pi} \approx 1.29 \). For a square-shaped inclusion, or \( n = 4 \), \( L_0 s / 2 \sqrt{\pi f} = 2 / \sqrt{\pi} \approx 1.13 \). Therefore, for a fixed phase-volume fraction \( f \), a triangular inclusion and a square-shaped inclusion will have 29% and 13% more interfacial area than a circular inclusion, respectively.

![Figure 8: Variation of the normalized specific surface as a function of the number of edges of the regular polygon-shaped inclusions: (a) for single inclusion, (b) for multiple non-overlapping inclusions.](image)

Among all the composite theories based upon the notion of a unit cell, square-shaped and circular inclusions are the favored choices. As shown in Fig. 8(a), the difference of the amount of interface area for these two favorite geometries is approxi-
mately 13%. If the interfacial behavior dominates the deformation process, this difference could yield an error when we attempt to predict the constitutive response of the heterogeneous composite.

It is also possible to consider unit cells with multiple inclusions. In Fig. 8(b), we plot the variation of the normalized specific surface, \( \frac{L_0 s}{2 \sqrt{\pi f}} \), as a function of the number of edges of the regular polygon-shaped inclusion for a different number of inclusions in the unit cell. We assume that all inclusions in the unit cell are identical and do not overlap. For a given inclusion phase-volume fraction, \( f \), and for a fixed number of edges of the regular polygon, the specific surface of a unit cell scales as a function of \( \sqrt{N} \), where \( N \) is the total number of inclusions in the unit cell. This very simple two-dimensional example demonstrates that the specific surface varies for different inclusion shapes and for different numbers of inclusions in a unit cell over a significant range, even when the inclusion phase-volume fraction is kept constant.

We focused on the detailed two-dimensional analysis above for the purpose of subsequently estimating the specific surface of PBX 9501. To generate such an estimate, we need to use the material’s optical micrographs, where the inclusions are objects with two-dimensional geometries. Nevertheless, we have also considered a cubic three-dimensional unit cell, in which the inclusion has the shape of a polyhedron (i.e., a three-dimensional object whose surface is composed of identical regular polygons).

Figure 9 shows six different polyhedron shapes: tetrahedron, cube, octahedron, dodecahedron, icosahedron, and sphere. The sphere is a special type of a polyhedron in which the number of faces grows toward infinity, whereas the surface area and the volume remain finite. In the three-dimensional case, the normalized specific surface becomes \( \frac{L_0 s}{(4 \pi)^{1/3} (3f)^{2/3}} \), which equals unity for a sphere. Once again, \( f \) denotes the inclusion phase-volume fraction of the unit cell. The normalized specific surface of three-dimensional polyhedron varies with the number of faces similarly
Figure 9: Variation of the normalized specific surface as a function of the number of faces of the polyhedron-shaped inclusion.

to the two-dimensional polygon. These results are shown in Fig. 8(a). Again, most composite theories use either cubic- or sphere-shaped inclusions. As shown in Fig. 9, however, for a given inclusion phase-volume fraction, the unit cell with a cubic inclusion has 24% more interfacial area than the unit cell with a spherical inclusion. We also studied three-dimensional unit cells with multiple inclusions of the same shape. In the three-dimensional case, for a given inclusion phase-volume fraction \( f \) and for a fixed number of faces of the polyhedron, the specific surface of a unit cell scales as a function of \( N^{1/3} \), where once again \( N \) represents the total number of non-overlapping inclusions in the unit cell.

In summary, even for very simple geometries the specific-surface value can vary over a very large spectrum. Such a large variation in the amount of interface area may introduce error in predicting the constitutive response of a heterogeneous composite, particularly if only the inclusion phase-volume fraction is considered when constructing the unit cell. Therefore, we should consider the inclusion phase-volume fraction

\[ \frac{L_0 s}{(4\pi^{1/3}(3f)^{2/3}} \]

\( n \rightarrow \infty \)

\[ \text{Tetrahedron} \]

\[ \text{Cube} \]

\[ \text{Octahedron} \]

\[ \text{Dodecahedron} \]

\[ \text{Icosahedron} \]

\[ \text{Sphere} \]
and the specific surface as two independent parameters that characterize a heterogeneous materials’s microstructure.

In the next section, we will show that for PBX 9501 it almost becomes impossible to construct a unit cell capable of capturing both the inclusion phase-volume fraction and the specific surface of the material. As a result, we must seek a new theoretical framework for developing constitutive models for heterogeneous composites, such as PBX 9501.

6 Measuring the Specific Surface of PBX 9501

We have shown that the specific surface, just like the phase-volume fractions, plays an important role in characterizing the microstructural morphology of any heterogeneous composite. One of the reasons that most composite theories use only the phase-volume fraction as the primary parameter is that it can be measured very accurately and easily. For a two-phase heterogeneous composite, the volume fraction of the inclusion phase is simply

\[ f_1 = \frac{1}{\rho_1 - \rho_2} \left( \frac{m}{V} - \rho_2 \right), \]  

(6.1)

where \( \rho_1 \) and \( \rho_2 \) are the mass densities of the inclusion phase and the matrix phase, respectively. We can measure the mass and the volume of the composite sample, \( m \) and \( V \) in equation (6.1), very accurately using simple laboratory equipment, such as a scale and a ruler.

However, conventional laboratory equipment cannot easily measure the specific surface or other microstructural quantities. Consequently, we need to employ more elaborate and advanced experimental techniques. One such technique is X-ray computed microtomography, which has been used successfully in obtaining three-dimensional microstructural images of some heterogeneous materials like sandstone and plastic foams. Unfortunately, in its current state this technique cannot resolve sub-
micron details, an essential feature of high explosives. We have to rely on optical microscopy and two-dimensional micrographs of the high explosive. Figure 10 shows such a micrograph of PBX 9501.

![Micrograph of PBX 9501](image)

Figure 10: Micrograph of PBX 9501 (courtesy of Paul Peterson, Dynamic Experimentation Division, and Bernd Schlei, Theoretical Division, of Los Alamos National Laboratory).

A digital gray-scale image (i.e., a mosaic of very small areas called pixels, with each pixel value corresponding to the average brightness of the object over that small area) forms the micrograph of a high explosive. The number of bits used for each pixel determines how many different brightness levels are available. The typical image contains 8 bits/pixel data, which corresponds to 256 (0–255) different brightness (gray) levels. To extract the microstructural information from the micrograph, however, we need to segment the image. The segmentation process finds regions that represent objects or meaningful parts of objects.

For a two-phase heterogeneous composite like PBX 9501, we need to separate regions occupied by the inclusion (energetic crystal) and the matrix (polymeric binder). To segment an image, we can use binarization, which is commonly done through thresholding. However, more sophisticated image segmentation algorithms are needed because PBX 9501 and other high explosives contain not only very coarse crystals in
the range of several hundred microns but also very fine particles or features in the range of submicrons. Recently, Schlei et al. (2000) developed a methodology that can obtain more accurate morphological information from micrographs of PBX 9501. Figure 10 is such a binary image, where white pixels show the region occupied by the HMX crystal and the black pixels represent a region occupied by the polymeric binder. Figure 10 contains visible long black scratch lines, which may be the result of polishing during sample preparation. As the algorithm evolves, we can expect to obtain higher-quality binary images for the morphological analysis.

We estimated the specific surface $s$ of PBX 9501 based on the two-point correlation function, $p_2(r)$, and the relation (4.6). To determine the two-point correlation function $p_2(r)$ from the micrograph, we employed a brute-force approach. For a given image with $n_x$ pixels in the $x$-direction and $n_y$ pixels in the $y$-direction, any point (or pixel), $p_{ij}$, within the image region is given by the coordinate $(i, j)$, $1 \leq i \leq n_x$ and $1 \leq j \leq n_y$. Now we can find all possible pairs of points, $(p_{ij}, p_{mn})$, in the region, where $1 \leq i, m \leq n_x$ and $1 \leq j, n \leq n_y$. These pairs may include $(p_{ij}, p_{ij})$; however, $(p_{ij}, p_{mn})$ and $(p_{mn}, p_{ij})$ represent the same pair and thus only one is counted. Assume that $N(r)$ is the total number of pairs, where the distance between the two end points is $r$, and that among these, $N_{\text{white}}(r)$ is the number of pairs where both end points of the pair fall in the region occupied by the crystal (i.e., both pixels are white). Then, according to its probabilistic interpretation, the two-point correlation function $p_2(r)$ is simply given by

$$p_2(r) = \frac{N_{\text{white}}(r)}{N(r)}, \quad r \geq 0. \quad (6.2)$$

Although this brute-force approach is quite straightforward, especially in terms of coding, the tremendous number of possible pairs in the image region represents a difficult issue. For example, if the image has $n_x = n_y = 64$ pixels, then the total number of possible pairs is $n_x n_y (n_x n_y + 1)/2 = 8,390,656$. As a result, we would need 10,000 GB of storage to handle an image that is $1000 \times 1000$ pixels in size. However,
we only need the behavior of the two-point correlation function $p_2(r)$ near $r = 0$. Thus, we only need to find all possible pairs that have a distance between points that is smaller than $r_0$. In such cases, we chose $r_0$ so that the behavior of $p_2(r)$ near $r = 0$ can be determined sufficiently well. Nevertheless, on a personal computer with a moderate amount of physical memory, we found that we can analyze an image with $128 \times 128$ pixels in size within a reasonable amount of time.

Figure 11 shows the result of analyzing a $128 \times 128$ pixels image. In Fig. 11(a), the microstructure of PBX 9501 is shown, where white pixels represent the HMX crystal and black pixels represent the polymeric binder. By using the procedure described above, for a given distance $r$, we can determine $p_2(r)$, which is presented as red dots in Fig. 11(b). A polynomial plotted as the solid blue line in the figure fits the red dots.

Figure 11: Determination of the two-point correlation function $p_2(r)$ of a $128 \times 128$ pixels image.

We calculated the slope of the two-point correlation function $p_2(r)$ at point $r = 0$, and it is drawn as the straight green line in Fig. 11(b). The specific surface of the image shown in Fig. 11(a) is given by

$$ s = -\pi \left\{ \frac{dp_2(r)}{dr} \bigg|_{r=0} \right\}. $$ (6.3)
If the image is larger than $128 \times 128$ pixels, it can be partitioned into several $128 \times 128$ sub-images. Equation (6.3) determines the specific surface of the sub-image, say $s_i$ ($i = 1, 2 \cdots, M$). In this case, $M$ is the total number of sub-images. The specific surface of the original image can be calculated from

$$s = \frac{\sum_{i=1}^{M} A_i s_i}{\sum_{i=1}^{M} A_i},$$

(6.4)

where $A_i$ is the area of the sub-image. We have assumed that the microstructure of each sub-image is random, so that the notion of two-point correlation function $p_2(r)$ and equation (4.6) are both valid.

We then applied our procedure to the four PBX 9501 micrographs shown in Fig. 12. These four images, each $1024 \times 1024$ pixels in size, were selected from different regions in Fig. 10. We first partitioned each $1024 \times 1024$ pixels image into 64 sub-images whose size was $128 \times 128$ pixels. The specific surface of each sub-image was determined according to equation (6.3) and then combined to specify the specific surface of the complete image using equation (6.4). The results were plotted and appear in Fig. 13.

To compare with the observations shown in Fig. 8, we plotted the normalized specific surface, $L_0s/2\sqrt{\pi f}$, in Fig. 13, where $L_0$ is the size of the image and $f$ is the volume fraction of the crystal (HMX) phase. The volume fractions of HMX were measured using Figs. 12(a)–12(d) as well. The dotted line in Fig. 13 locates the mean value of our results from the four different images. Recall that if a unit cell, with the size of $L_0$, contains only one circular inclusion with the volume fraction $f$, the normalized specific surface, $L_0s/2\sqrt{\pi f}$, equals one. Thus, the normalized specific surface determined from the micrographs in Fig. 12 of PBX 9501 is significantly greater than unity. In other words, any unit cell we can conceivably construct based on simple geometries, will grossly underestimate the amount of interface area in PBX 9501.

Another observation can be made from Fig. 13. The four arbitrarily chosen images

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*Specific Surface: A Missing Parameter in High-Explosive Modeling*
in Fig. 12 have different values of the normalized specific surface, as shown in Fig. 13. This phenomenon results from the notion of the minimum representative volume element (RVE) for PBX 9501. The minimum RVE defines a length scale above which the heterogeneous material can be viewed as homogeneous. In other words, the response of all the material elements, whose sizes are larger than the minimum RVE, will be the same under the same external loading conditions. Below the length scale of the minimum RVE, the material elements exhibit a statistical characteristic related to the material’s heterogeneous nature. The scatter of the specific-surface results (as shown
Figure 13: Normalized specific surface of PBX 9501.

in Fig. 13) indicates that the material elements, as shown in Figs. 12(a)–12(d), are still smaller than the minimum RVE of PBX 9501. Liu et al. (2002) experimentally studied the minimum RVE size of the PBS 9501, a sugar-mock simulant of PBX 9501, using the digital-image correlation technique. Based on the mechanical response of the material, Liu et al. estimated that the minimum RVE of the sugar-mock material is about 1.5 mm.

7 Discussion

Using a simple example, we have shown that we must model high-explosive materials as multiphase composites so that we can capture damage initiation and evolution. Because of the material’s extremely complicated microstructure, phase-volume fractions alone cannot characterize the microstructure. We believe that the so-called specific surface (i.e., interfacial area per unit volume) is an additional parameter to use. We also believe that it is best to consider both the phase-volume fraction and the specific surface as primary and independent parameters for describing the microstructural characteristics of high explosives. To estimate the value of the specific surface, we used a

\[ L_0 s f / 2 \sqrt{\frac{\pi}{f}} \]

\[ 0 \quad 10 \quad 20 \quad 30 \quad 40 \quad 50 \]

Image A Image B Image C Image D

\(^1\)While preparing this section, I benefited greatly from illuminating discussions with Professor Young Huang of the Department of Mechanical & Industrial Engineering, University of Illinois at Urbana-Champaign.
new methodology that takes advantage of data provided by a binarized micrograph of PBX 9501. The basis of our new method consists of (1) the two-point correlation function and (2) the assumption that PBX 9501 possesses a random microstructure. Our preliminary study indicates that the conventional way of constructing the unit cell (an approach advocated by many existing composite theories) would grossly underestimate the specific surface of the high explosive. Consequently, these theories may underestimate the contribution from the interface to the overall mechanical response of the high explosive.

Figure 14 illustrates our overall strategy used to establish constitutive models of high explosives. First, a constitutive model for the constituents is required. An energetic crystal and a polymeric binder make up a two-phase high explosive. We must also characterize the constitutive behavior of the interface between the energetic crystal and the polymeric binder. Once the three components are known, we can formulate a theoretical framework that ties the components together. At this stage, the microstructural information is usually “hard-wired” into the theoretical framework. All the components within the light gray area in Fig. 14 comprise a composite theory. This theory will clarify the interactions between all the constituent phases and interfaces. A final constitutive model results from the combination of the composite theory and the detailed information about the constitutive behavior of all the constituents and interfaces.

Even though all the components shown in Fig. 14 are equally important, we believe that the most challenging task is the development of a composite theory. All existing composite theories place equal importance on the top three boxes shown in Fig. 14. However, in terms of the amount of contribution from each component, most composite theories consider the first two as primary and the third one as secondary. This is why the unit cell is typically constructed by using only the phase-volume fractions. For composites with simple microstructures, such approaches have proven successful. However, because composites like PBX 9501 have complicated microstructures, such
oversimplification, coupled with ignoring the microstructural information, handicaps the approach.

The high magnitude of the specific surface we calculated for PBX 9501 may be unattainable with the unit-cell methodology. Of course, we could try to construct such a cell representing both the phase-volume fraction and the specific surface. But from an engineering point of view, such an attempt would not produce a constitutive model that is numerically efficient and cost effective.

We envision a method that incorporates both volume fraction and specific surface, but that does not rely on the notion of a unit cell. Making significant contributions to this effort was Professor Young Huang, Department of Mechanical and Industrial Engineering, University of Illinois at Urbana-Champaign. The premise of our approach is that instead of solving detailed stress or strain distributions among different phases and the interface, we study how the total energy caused by external loading is distributed among the constituent phases and the interface. As part of this approach, we employ the generalized Budiansky’s energy-equivalence framework (Budiansky, 1965).
Consider a material element, \( R \), of a two-phase composite, where the volume of the element is \( V \). The element \( R \) is the union of two disjoint subelements, \( R_1 \) and \( R_2 \), with volumes \( V_1 = f_1 V \) and \( V_2 = f_2 V \), respectively, where \( f_1 \) and \( f_2 \) are the phase-volume fractions and \( f_1 + f_2 = 1 \). The element has an interfacial area between the two phases of \( S_{\text{int}} = s V \), where \( s \) is the composite’s specific surface. We assume that the microstructure within this material element is random and that the spatial distribution of the different phases is such that the response of the composite material is homogeneous, provided that the material elements are big enough (larger than the so-called minimum RVE). Also, for now we assume that the deformation of the two phases and the composite are all elastic. As a result, the stress-strain relations for the constituents become

\[
\sigma_{ij} = C_{ijkl}^{(a)} \epsilon_{kl}, \quad \text{or} \quad \epsilon_{ij} = B_{ijkl}^{(a)} \sigma_{kl} \quad a = 1, 2,
\]

and for the composite,

\[
\Sigma_{ij} = C_{ijkl} E_{kl}, \quad \text{or} \quad E_{ij} = B_{ijkl} \Sigma_{kl}.
\]

In the above, \( C_{ijkl} \) denotes the elastic stiffness, \( B_{ijkl} \) the elastic compliance, and

\[
C_{ijkl} B_{mnkl} = \frac{1}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \equiv I_{ijkl},
\]

is the fourth-order identity tensor. Now, apply a uniform traction \( t_i = \Sigma_{ij} n_j \) on the surface of the material element \( R \), where \( n_i \) is the outward unit normal vector along the surface of \( R \). The strain energy of the composite material element \( R \) is exactly given as

\[
U = \frac{1}{2} B_{ijkl} \Sigma_{ij} \Sigma_{kl} V,
\]

where, once again, \( V \) is the volume of the material element \( R \). In terms of the stresses and strains in various phases and along the interface,

\[
U = \frac{1}{2} \int_V \sigma_{ij} \epsilon_{ij} \, dV + \frac{1}{2} \int_{S_{\text{int}}} \sigma_{ij} n_i [u_j] \, dA,
\]
where \([u_i] = u_i^+ - u_i^-\) is the displacement jump across the interface and \(n_i\) is the unit normal vector along the interface. In writing equation (7.4), we adopt the convention that the phase 2 side of the interface is denoted as (+) and the phase 1 side of the interface is (−). Thus, the normal \(n_i\) points from the (−) side to the (+) side.

Now, we further manipulate the first term in equation (7.4),

\[
\frac{1}{2} \int_V \sigma_{ij} \epsilon_{ij} \, dV = \frac{1}{2} \int_{V_1} \sigma_{ij}^{(1)} \epsilon_{ij}^{(1)} \, dV + \frac{1}{2} \int_{V_2} \sigma_{ij}^{(2)} \epsilon_{ij}^{(2)} \, dV
\]

\[
= \frac{1}{2} \int_{V_1} \sigma_{ij}^{(1)} u_{j,i} \, n_i \, dV + \frac{1}{2} \int_{V_2} \sigma_{ij}^{(2)} u_{j,i} \, n_i \, dV
\]

\[
= \frac{1}{2} \int_{S_{\text{out}}} \sigma_{ij}^{(1)} u_j^{(1)} n_i \, dA + \frac{1}{2} \int_{S_{\text{out}}} \sigma_{ij}^{(2)} u_j^{(2)} n_i \, dA + \frac{1}{2} \int_{S_{\text{int}}} \sigma_{ij}^{(1)} u_j^{(1)} n_i^{(1)} \, dA + \frac{1}{2} \int_{S_{\text{int}}} \sigma_{ij}^{(2)} u_j^{(2)} n_i^{(2)} \, dA,
\]

where \(S_\alpha (\alpha = 1, 2)\) is the total bounding surface of \(R_\alpha\). It is easy to see that \(S_\alpha = S_{\text{out}}^{(a)} + S_{\text{in}}^{(a)}\), where \(S_{\text{out}}^{(a)}\) is part of the outside surface of material element \(R\) that comes from phase \(\alpha\). In the above derivation, we have used the strain-displacement relation \(\epsilon_{ij} = (u_{i,j} + u_{j,i})/2\), symmetry of the stress tensor \(\sigma_{ij} = \sigma_{ji}\), equilibrium of the stress field \(\sigma_{i,j} = 0\), and the divergence theorem. Note that along the interface \(S_{\text{int}}\), we have \(\sigma_{ij}^{(1)} = \sigma_{ij}^{(2)}\), \(u_{j}^{(1)} = u_{j}^{(2)}\), \(u_{i}^{(1)} = u_{i}^{(2)}\), and \(n_{i}^{(1)} = -n_{i}^{(2)} = n_{i}\), according to the conventions outlined above. As a result,

\[
\frac{1}{2} \int_{S_{\text{int}}} \sigma_{ij}^{(1)} u_j^{(1)} n_i^{(1)} \, dA + \frac{1}{2} \int_{S_{\text{int}}} \sigma_{ij}^{(2)} u_j^{(2)} n_i^{(2)} \, dA = \frac{1}{2} \int_{S_{\text{int}}} \sigma_{ij} n_i [u_j] \, dA.
\]

Therefore, equation (7.4) becomes

\[
U = \frac{1}{2} \int_{S_{\text{out}}}^{(1)} \sigma_{ij} u_j^{(1)} n_i \, dA + \frac{1}{2} \int_{S_{\text{out}}}^{(2)} \sigma_{ij} u_j^{(2)} n_i \, dA.
\]

(7.5)

On the outside surface of \(R\), \(\sigma_{ij} n_i = t_i = \Sigma_{ij} n_i\), according to the prescribed boundary condition. Therefore, equation (7.5) can be written as

\[
U = \frac{1}{2} \Sigma_{ij} \int_{S_{\text{out}}}^{(1)} u_j^{(1)} n_i \, dA + \frac{1}{2} \Sigma_{ij} \int_{S_{\text{out}}}^{(2)} u_j^{(2)} n_i \, dA.
\]

(7.6)
We can also show that

\[
\Sigma_{ij} \int_{S_{\text{out}}} u_{i}^{(1)} n_{i} \, dA = \Sigma_{ij} \int_{S_{1}} u_{i}^{(1)} n_{i} \, dA - \Sigma_{ij} \int_{S_{\text{int}}} u_{i}^{(1)} n_{i} \, dA \\
= \Sigma_{ij} \int_{V_{1}} u_{i}^{(1)} n_{i} \, dV - \Sigma_{ij} \int_{S_{\text{int}}} u_{i}^{(1)} n_{i} \, dA = \Sigma_{ij} \int_{V_{1}} \epsilon_{ij}^{(1)} \, dV - \Sigma_{ij} \int_{S_{\text{int}}} u_{i}^{+} n_{i} \, dA,
\]

where \( \Sigma_{ij} = \Sigma_{ji} \) has been used, and similarly

\[
\Sigma_{ij} \int_{S_{\text{out}}} u_{j}^{(2)} n_{i} \, dA = \Sigma_{ij} \int_{V_{2}} \epsilon_{ij}^{(2)} \, dV + \Sigma_{ij} \int_{S_{\text{int}}} u_{i}^{+} n_{i} \, dA.
\]

Consequently, equation (7.6) becomes

\[
U = \frac{1}{2} \Sigma_{ij} \int_{V} \epsilon_{ij} \, dV + \frac{1}{2} \Sigma_{ij} \int_{S_{\text{int}}} \| u_{j} \| n_{i} \, dA. \tag{7.7}
\]

From identity, strain \( \epsilon_{ij} \) can be decomposed into

\[
\epsilon_{ij} = B_{ijkl}^{(2)} \sigma_{kl} + (\epsilon_{ij} - B_{ijkl}^{(2)} \sigma_{kl}),
\]

where \( B_{ijkl}^{(2)} \) is the elastic compliance of the second phase and \( \sigma_{ij} \) is the stress in various phases. Therefore, the stress is nonuniform in the volume. The strain energy in equation (7.7) becomes

\[
U = \frac{1}{2} B_{ijkl}^{(2)} \Sigma_{ij} \int_{V} \sigma_{kl} \, dV + \frac{1}{2} \Sigma_{ij} \int_{V} (\epsilon_{ij} - B_{ijkl}^{(2)} \sigma_{kl}) \, dV + \frac{1}{2} \Sigma_{ij} \int_{S_{\text{int}}} \| u_{j} \| n_{i} \, dA. \tag{7.8}
\]

The first integral in equation (7.8) can be rearranged to be

\[
\int_{V} \sigma_{kl} \, dV = \int_{V} \sigma_{ml} \delta_{km} \, dV = \int_{V} \sigma_{ml} x_{km} \, dV = \int_{V} (\sigma_{ml} x_{k})_{m} \, dV \\\n= \int_{S} \sigma_{ml} n_{m} x_{k} \, dS = \Sigma_{ml} \int_{S} n_{m} x_{k} \, dS = \Sigma_{ml} \int_{V} x_{km} \, dV = \Sigma_{ml} \delta_{km} \int_{V} \, dV = \Sigma_{kl} V,
\]

where \( x_{i} \) is the Cartesian coordinate. The constitutive relation for phase 2 in equation (7.1) requires the integrand in the second integral in equation (7.8) to be identically zero over the region \( R_{2} \). Hence, the second integral becomes

\[
\int_{V_{1}} \{ \epsilon_{ij}^{(1)} - B_{ijkl}^{(2)} \sigma_{kl}^{(1)} \} \, dV = \left\{ \frac{1}{2} (\delta_{im} \delta_{jn} + \delta_{in} \delta_{jm}) - B_{ijkl}^{(2)} C_{klmn}^{(1)} \right\} \int_{V_{1}} \epsilon_{mn}^{(1)} \, dV \\\n= f_{1} \left\{ \frac{1}{2} (\delta_{im} \delta_{jn} + \delta_{in} \delta_{jm}) - B_{ijkl}^{(2)} C_{klmn}^{(1)} \right\} \epsilon_{mn}^{(1)} V,
\]
where we have used the relation \( V_1 = f_1 V \), and \( f_1 \) is the volume fraction of phase 1. Meanwhile, we defined
\[
\varepsilon_{mn}^{(1)} = \frac{1}{V_1} \int_{V_1} \varepsilon_{mn}^{(1)} \, dV
\]
as the average strain in phase 1. Similarly, the last integral in equation (7.1) can be written as
\[
\Sigma_{ij} \int_{S_{int}} [u_j] n_i \, dA = s \Sigma_{ij} \varepsilon_{ij}^{\text{int}} \Sigma_{ij} \varepsilon_{ij}^{\text{int}} V,
\]
where
\[
\varepsilon_{ij}^{\text{int}} = \frac{1}{2S_{int}} \int_{S_{int}} ([u_i] n_j + [u_j] n_i) \, dA,
\] (7.9)
which is the average strain due to the deformation along the interface between the two phases. To reach this result, we have used the relation \( S_{int} = s V \). Finally, the strain energy in equation (7.1) becomes
\[
U = \frac{V}{2} \left\{ B_{ijkl}^{(2)} \Sigma_{ij} \Sigma_{kl} + f_1 \left( \frac{\delta_{im} \delta_{jn} + \delta_{in} \delta_{jm}}{2} - B_{ijkl}^{(2)} C_{klmn}^{(1)} \right) \Sigma_{ij} \varepsilon_{mn}^{(1)} + s \Sigma_{ij} \varepsilon_{ij}^{\text{int}} \right\}. \tag{7.10}
\]
Equation (7.10) represents contributions from various constituents to the overall strain energy of the material element. We see that the strain energy depends explicitly on both the phase-volume fraction, \( f_1 \), and the specific surface \( s \). Therefore, this formulation appropriately accounts for the contributions to the total strain energy from the two different phases, as well as the interface between the two phases. An interesting feature of the above representation is worth mentioning. By recalling the definition of the average strain \( \varepsilon_{ij}^{\text{int}} \) in (7.9), we see that if the bonding between the two constituent phases is perfect (i.e., \([u_i] \equiv 0 \) for \( i = 1, 2, 3 \)), then \( \varepsilon_{ij}^{\text{int}} \equiv 0 \). As a result, the strain energy, as shown in (7.10), no longer depends on the specific surface \( s \).

By comparing equations (7.3) and (7.10), we find
\[
B_{ijkl} \Sigma_{ij} \Sigma_{kl} = B_{ijkl}^{(2)} \Sigma_{ij} \Sigma_{kl} + f_1 \left( \frac{\delta_{im} \delta_{jn} + \delta_{in} \delta_{jm}}{2} - B_{ijkl}^{(2)} C_{klmn}^{(1)} \right) \Sigma_{ij} \varepsilon_{mn}^{(1)} + s \Sigma_{ij} \varepsilon_{ij}^{\text{int}}. \tag{7.11}
\]
Note that the equation (7.11) is the exact representation of the energy equivalence, and that there is no assumption made for establishing this relationship.
To further illustrate the framework presented by equation (7.11), we invoke linearity of the problem. Therefore, there must exist the following relationships:

$$
\varepsilon^{(1)}_{ij} = M^{(1)}_{ijkl} \Sigma_{kl}, \quad \varepsilon^{\text{int}}_{ij} = M^{\text{int}}_{ijkl} \Sigma_{kl}.
$$

(7.12)

Different methods can be used to establish the fourth-order tensors $M^{(1)}_{ijkl}$ and $M^{\text{int}}_{ijkl}$, and different degrees of approximation may be introduced at this stage. By substituting equation (7.12) into equation (7.11), we have

$$
B_{ijkl} \Sigma_{ij} \Sigma_{kl} = \left\{ B^{(2)}_{ijkl} + f_1 \left( \frac{\delta_{im} \delta_{jn} + \delta_{in} \delta_{jm}}{2} - B^{(2)}_{ijpq} C^{(1)}_{pqmn} \right) M^{(1)}_{mnkl} + s M^{\text{int}}_{ijkl} \right\} \Sigma_{ij} \Sigma_{kl}.
$$

(7.13)

This is a quadratic equation of $\Sigma_{ij}$. There are 21 quadratic terms, such as $\Sigma_{11}^2$ and $\Sigma_{11} \Sigma_{12}$. Comparing the coefficients of these 21 terms in equation (7.13) leads to 21 equations. From these equations, we can completely determine the 21 components of the elastic compliance of the composite, $B_{ijkl}$. This framework differs distinctly from other composite theories. The elastic compliance $B_{ijkl}$, or the stiffness $C_{ijkl}$, depends not only on the elastic constants of the constituent phases and the volume fractions, but also on the behavior of the interface, through the tensor $M^{\text{int}}_{ijkl}$ and the amount of interface, through the parameter $s$.

We need to point out that the energy equivalence of equations (7.3) and (7.4) is just a special case of the modified basic lemma (3.16). In such a special case, we required that the local stress $\sigma$ and the local strain $\epsilon$ satisfy an elastic relationship. We also required that the macroscopic stress $\Sigma$ is a homogeneous linear function of the macroscopic strain $E$. However, in the modified basic lemma (3.16), the local stress $\sigma$ and the local strain $\epsilon$, as well as the macroscopic stress $\Sigma$ and the macroscopic strain $E$, are not necessarily related by a constitutive relation. If we replace $\sigma$, $\epsilon$, $\Sigma$, and $E$ in equation (3.16) by their corresponding incremental forms and carry out the derivation discussed above, then equation (7.13) actually specifies the relationship between the tangential compliance of the material element and the tangential compliances and tangential stiffness of the constituent phases, as well as the interface. As a result, it is
quite straightforward to extend the energy-equivalence framework to analyze nonlinear responses of high explosives.

This energy-equivalence framework offers several advantages over other theories. First, we do not require a unit cell, which may substantially improve computational efficiency. And second, by explicitly accounting for the exact amount of interface, we accurately represent the underlying physics of deformation. This is also the ultimate goal that we are trying to achieve. This framework presents some additional advantages, which it may share with other formulations. Our composite theory has a modular structure, as illustrated in Fig. 14, and thus we can concentrate on different phases of the composite for different mechanisms. For example, to address damage and cracking, chemical reactions, and hot-spot development, our models can concentrate exclusively on the energetic crystal, rather than on the entire composite. The SCRAM model is an ideal candidate for this module (Dienes, 1996). For viscoelastic deformation and aging, the analysis should focus on the polymeric binder (Clements and Mas, 2001a and 2001b; Zhang et al., 2002). A third effort would lead to a better description of the interface between phases. We can plug each separate piece into the framework to customize a constitutive model for the high explosive.

Our current framework can easily address an issue that other composite theories may find difficult to tackle. To ensure a composite theory’s validity, we must consider a material element that is larger than the minimum representative volume element. Above this length scale, the composite responds homogeneously; below this length scale, the material exhibits statistical characteristics as a result of its heterogeneous nature. There may be occasions in which we need to consider material elements that are smaller than the minimum RVE. Because of the statistical nature of the response, we do not need to know the exact value of the deformation, but we must know the mean value of the deformation and the magnitude of the fluctuation of the deformation. The framework we presented in this section offers an easy way to estimate the mean value and the fluctuations. We can write our composite theory in the following
way:

$$
\sigma_{ij} = F_{ij}(\epsilon, \dot{\epsilon}, T, C^{(1)}, C^{(2)}, M^{(1)}, M^{\text{int}}, \cdots ; f_1, s). \tag{7.14}
$$

The fluctuation of the stress $\delta \sigma_{ij}$ can be estimated by

$$
\delta \sigma_{ij} = \frac{\partial F_{ij}}{\partial f_1} \delta f_1 + \frac{\partial F_{ij}}{\partial s} \delta s. \tag{7.15}
$$

In this equation, we attribute the fluctuation of the stress to variations in the parameters $f_1$ and $s$. The heterogeneous nature of the microstructure produces these fluctuations. From the micrograph, we can measure the volume fraction $f_1$ and the specific surface $s$, quantifying the fluctuations of $f_1$ and $s$ as a function of different material element sizes in the process. Because our energy-equivalence framework, represented by the equation (7.11), depends explicitly on the volume fraction and the specific surface, the derivatives in (7.15) can be easily evaluated. Therefore, we can apply equations (7.14) and (7.15) to estimate the mean value and the magnitude of stress fluctuations for a material element smaller than the minimum RVE.

In this section, we presented some general ideas of how to establish a composite theory based on the energy-equivalence framework. Some unique features and advantages of this framework were discussed. For demonstration purposes, to date we have only considered a linearly elastic case. However, it is possible to extend the framework to nonlinear cases. We believe that extending this effort to further develop the framework is worthwhile, and we are thus continuing the effort.

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