

# EFFECTIVE ELASTIC PARAMETERS OF CARBON/CARBON COMPOSITES WITH NON-ELLIPSOIDAL PORES

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## 1 Introduction. Cavity Compliance Tensor

We present a homogenization procedure to predict the effective elastic properties of materials containing randomly distributed non-ellipsoidal pores. Such materials can be either isotropic or anisotropic depending on the elastic symmetry of matrix material and orientational distribution of defects. The approach is based on the evaluation of compliance contribution tensor of each pore type [1]. For some pore types this can be done analytically utilizing existing elasticity solution [2, 3]. The examples of such geometries are 3D ellipsoids, 2D ellipses and equilateral polygons. However, there are no convenient analytical solutions for irregular pore shapes, so that numerical techniques, e.g. finite element method (FEA), have to be used. The FEA procedure to determine the cavity compliance contribution tensor of an arbitrarily shaped cavity in some isotropic or anisotropic matrix is presented in section 2.

The fourth rank compliance contribution tensor  $\mathbf{H}$  of an individual cavity is defined as a set of proportionality coefficients between remotely applied homogeneous stress field  $\boldsymbol{\sigma}^{(0)}$  and the additional strain  $\Delta\boldsymbol{\varepsilon}$  generated in the material due to the presence the cavity:

$$\Delta\boldsymbol{\varepsilon} = \mathbf{H} : \boldsymbol{\sigma}^{(0)}. \quad (1)$$

The choice of micromechanical model used to predict the effective elastic properties of material with many pores depends on their concentration. If pores are sufficiently away from each other (dilute limit), the non-interaction approximation can be used. We choose the proper representative volume element (RVE) [4, 5], and calculate the overall

compliance contribution tensor for the RVE by direct summation:

$$\mathbf{H}_{RVE}^{NI} = \sum \mathbf{H}^{(i)}, \quad (2)$$

where  $\mathbf{H}^{(i)}$  is the compliance contribution tensor of an individual pore, and the summation is performed over all defects present in the RVE. Denoting by  $\mathbf{S}^{(0)}$  the compliance of the of matrix material, we obtain the following expession for the effective compliance tensor

$$\mathbf{S} = \mathbf{S}^{(0)} + \mathbf{H}_{RVE}^{NI}, \quad (3)$$

from which all effective elastic parameters of the porous material can be extracted.

For non-dilute distribution of pores, some more advanced micromechanical scheme can be used. For example, predictions for the overall elastic compliance by the Mori-Tanaka method [6] in terms of  $\mathbf{H}_{RVE}^{NI}$  is given by a simple formula

$$\mathbf{H}_{RVE}^{MT} = \mathbf{H}_{RVE}^{NI} / (1 - p), \quad (4)$$

where  $p$  is the volume fraction of pores [1].

## 2 Evaluation of Contribution of a Single Pore by Finite Element Analysis

The pore compliance contribution tensor of a non-ellipsoidal pore can be calculated numerically using FEA. The following procedure utilizing MSC.MARC ([www.mscsoftware.com](http://www.mscsoftware.com)) software package was implemented by the authors (for details see [7]):

(a) The pore surface is placed into the reference volume in the shape of a cube with sides five times larger than the largest dimension of the pore (Fig. 1).

This setup is auto meshed with tetrahedral 3D elements;

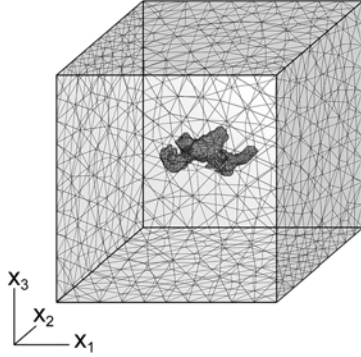


Fig.1. Reference volume and pore surface mesh

(b) To obtain all 21 independent components of  $\mathbf{H}$ -tensor, six loadcases (3 uniaxial tensions and 3 shear deformations in perpendicular directions) are considered;

(c) The FEA simulations are performed and the stress and strain fields are calculated;

(d) The components of the pore  $\mathbf{H}$ -tensor are calculated based on the average values of strain. For example, from the uniaxial tension in  $x_1$  direction  $\sigma_{11}^{(0)}$  we obtain:

$$H_{ij11} = \frac{S_{ij11}^{(0)} \sigma_{11}^{(0)} - \langle \varepsilon_{ij} \rangle_{RVE}}{\sigma_{11}^{(0)}}. \quad (5)$$




### 3 Results for Pores in Carbon/Carbon Composites

The above procedure was utilized to evaluate contribution of irregularly shaped 3D pores to the overall properties of carbon/carbon composites. The shapes of the pores were determined by X-ray computed microtomography [8]. As an example, Table 1 provides contributions of several pore shapes to the effective Young's moduli in the directions of coordinate axes. The parameters  $\tilde{E}_i$  presented in the table enter the expressions for the Young's moduli as

$$E_i = E^{(0)} / (1 + p \tilde{E}_i), \quad (6)$$

where  $p$  is the volume fraction of parallel pores of the corresponding shape.

Table1. Contributions of selected pores to the effective Young's moduli

Cavity shapes	$\tilde{E}_1$	$\tilde{E}_2$	$\tilde{E}_3$
	1.753	2.359	2.591
	1.711	2.674	2.176
	1.831	2.348	2.499

### 4 Approximation of Irregularly Shaped Pores by Ellipsoids

Traditionally in micromechanical analysis three-dimensional inhomogeneities are assumed to be ellipsoidal. This is done because only such shapes possess the property of uniform eigenstrain under remotely applied loading, so that the analytical solutions for strains and stresses around them can be utilized [2, 9].

For irregular defect shapes, one possible approach is to find the bounds of individual pore contributions by considering the inscribed and circumscribed ellipsoids constructed for such a pore [4, 10]. However, for the shapes considered in Table 1 of the previous section, such an approach would result in extremely wide bounds due to large differences between the dimensions of the inscribed and circumscribed ellipsoids.

When pores are approximated by ellipsoids, two major issues have to be addressed: the choice of the best approximation of real pore shape by an ellipsoid (orientations and lengths of principal axes) and accuracy of the chosen approximation. In this section of the paper, we propose a principal component analysis (PCA) approach [11] utilizing the experimentally obtained 3D  $\mu$ CT data to construct the approximating ellipsoids, and evaluate the accuracy of the approach in terms of effective property predictions.

In the presentation of PCA approach, the notation  $x, y, z$  for the point coordinates will be used. Processing the  $\mu$ CT data, the pores in the image

were labeled and the surface of the pores was extracted to obtain input points  $(x_i, y_i, z_i)$  for the estimation of geometrical properties using PCA. Additionally, the volume and center of mass of each pore were determined for further use in the fitting process. A statistical method for describing variations or similarities in data is given by the variance or covariance of a data set [11]. In our case, the data set is comprised of all the surface points of the pore, which are a reduced representation of the complete body of the pore structure. It is possible to simplify the description of a pore in the composite to be represented by only a few characteristic parameters by applying the PCA methods to the data set. Therefore, it is necessary to compute the variance in 3D points and assemble the covariance matrix of the pore with all the necessary information to describe a simplified representation of the pore geometry. The covariance of two sets of variables, for example  $(X, Y)$ , is defined as:

$$\text{cov}(X, Y) = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{n-1}. \quad (7)$$

For the direct estimation of the geometrical parameters of the pore in a local coordinate system, it is advantageous to subtract the center of mass  $(\bar{X}, \bar{Y}, \bar{Z})$  from each point in the point set before the covariance matrix is constructed. This sets the origin of the coordinate system to the center of mass and relates all geometrical parameters to the local coordinate system.

Using the definition of the covariance of the three dimension in space for the point set the covariance matrix is:

$$\mathbf{C} = \begin{bmatrix} \text{cov}(X, X) & \text{cov}(X, Y) & \text{cov}(X, Z) \\ \text{cov}(Y, X) & \text{cov}(Y, Y) & \text{cov}(Y, Z) \\ \text{cov}(Z, X) & \text{cov}(Z, Y) & \text{cov}(Z, Z) \end{bmatrix}. \quad (8)$$

This matrix is symmetric and, using the spectral theorem of linear algebra, we apply the eigenvector decomposition to rewrite the covariance matrix in the form:

$$\mathbf{C} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^T. \quad (9)$$

Matrix  $\mathbf{\Lambda} = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$  is the diagonal matrix of eigenvalues

$$\mathbf{\Lambda} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}, \quad (10)$$

where  $\sqrt{\lambda_1}$ ,  $\sqrt{\lambda_2}$  and  $\sqrt{\lambda_3}$  are the semi-axes of the approximating ellipsoid and  $\mathbf{Q}$  is the matrix of eigenvectors composed of the direction cosines of the ellipsoid's principal axes organized in columns. Thus, all parameters of the approximating ellipsoid are defined. The resulting surface has the same variance as the original set of surface data points.

## 5 Examples of Ellipsoidal Approximations of Pores in Carbon/Carbon Composite

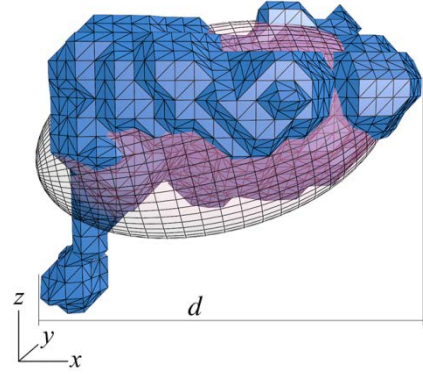


Fig. 2. Pore and approximating ellipsoid

Let us consider the pore shown in Fig. 2. Application of the procedure presented in section 4 results in the approximating ellipsoid with axes  $a = 0.347d$ ,  $b = 0.557d$ ,  $c = 0.972d$ , where  $d$  is the length of the pore in  $x$  direction. The Euler angles defining orientation of the ellipsoid ( $ZY'Z''$  convention) are  $-4.7^\circ$ ,  $76.7^\circ$  and  $-109.7^\circ$ , correspondingly.

Comparing the components of normalized  $\bar{\mathbf{H}}$ -tensor ( $\bar{\mathbf{H}} = \mathbf{H} \cdot E^{(0)} / p$ ) with the values for the original pore, we observe that diagonal terms are within 40% difference (1.865, 1.519 and 3.013 for the ellipsoid vs 1.4912, 2.765 and 2.117 for the original pore). No conclusive observation, however, for the off-diagonal terms can be made. Introducing the Euclidean norm of the 4<sup>th</sup> rank tensor  $\|\mathbf{S}\| = \sqrt{S_{ijkl} S_{ijkl}}$  (summation over the repeating indices), the relative

distance between the compliance contribution tensor of the actual pore and its approximation is




$$\Delta = \frac{\sqrt{(S_{ijkl}^{exact} - S_{ijkl}^{appr})(S_{ijkl}^{exact} - S_{ijkl}^{appr})}}{\sqrt{(S_{pqrs}^{exact} S_{pqrs}^{exact})}} = 0.33. \quad (11)$$

Note that this parameter is called error in [12], where authors utilized it to analyze elastic symmetries.

To provide a more mechanically meaningful comparison, Table 2 presents compressibility and shear compliance values for approximating ellipsoids compared to the corresponding parameters of the original shapes of the selected pores. These parameters are present in the expressions for effective bulk and shear moduli of materials with randomly oriented pores of a certain type:

$$K = K^{(0)} / (1 + p\tilde{K}), \quad G = G^{(0)} / (1 + p\tilde{G}). \quad (12)$$

Table 2. Parameters  $\tilde{K}$  and  $\tilde{G}$  for pores compared to their approximating ellipsoids

Pore	$\tilde{K}_p$	$\tilde{K}_{ELL}$	$\tilde{G}_p$	$\tilde{G}_{ELL}$
	5.117	4.970	1.932	1.934
	5.402	4.840	1.999	1.914
	5.354	4.782	1.992	1.901

The contribution of ellipsoids ( $\mathbf{H}$ -tensor) was found by utilizing the analytical solutions of Eshelby [2, 9].

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