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Prediction of the effective elastic moduli of materials with irregularly-shaped pores based on the pore projected areas

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ABSTRACT

Statistical modeling is used to correlate geometric parameters of pores with their contributions to the overall Young's moduli of linearly elastic solids. The statistical model is based on individual pore contribution parameters evaluated by finite element simulations for a small pore subset selected using the design of experiments approach, so there is no need to solve the elasticity problem for all pores in the material. A polynomial relating pore geometric parameters to the contribution parameters is then fitted to the results of the simulations. We found a good correlation between normalized projected areas of the pores on three coordinate planes and their contributions to the corresponding effective Young's moduli. The model is applied and validated for two large sets of pore geometries obtained by X-ray microcomputed tomography of a carbon/carbon and a 3D woven carbon/epoxy composite specimens.

1. Introduction

Effective stiffness of linear elastic solids is reduced by the presence of pores. Historically, this reduction has been quantified in terms of the relative volume fraction of pores (porosity) assuming all pores to be spherical, see Dewey (1947), Mackenzie (1950). Later, the pore shapes were included in consideration by utilizing the famous Eshelby solution (Eshelby, 1957, 1959) for ellipsoidal inclusions and modeling non-spherical pores as ellipsoids of various eccentricities, see Wu (1966) and discussions in Kachanov et al. (1994) and David and Zimmerman (2011). For two-dimensional pores, in addition to circular and elliptical shapes, the analytical solutions for various quazi-polygonal holes have been utilized, see Zimmerman (1986), Tsukrov and Kachanov (1993), Jasiuk et al. (1994), Kachanov et al. (1994), Ekneligoda and Zimmerman (2006, 2008b), Zou et al. (2010). In three-dimensional case, only a limited number of analytical solutions for non-ellipsoidal inhomogeneities are available, including cuboids (Lee and Johnson, 1978), polyhedra (Rodin, 1996; Nozaki and Taya, 1997; Lubarda and Markenscoff, 1998), and superspherical shapes (Onaka, 2001; Hashemi et al., 2009; Sevostianov and Giraud, 2012) To evaluate contributions of pores having irregular shapes, when no analytical solution for a given shape is available, various numerical techniques, such as finite element or boundary element analyses, can be used.

Direct micromechanical modeling is the preferred way to predict effective elastic properties of materials with pores (with other possibilities being variational bounds on a property as in Hashin and Shtrikman, 1962 and later publications, or finite element simulations for the entire representative volume element with many pores as in Roberts and Garboczi (2000), Arns et al. (2002) and González et al. (2004)). It involves evaluation of contribution of a certain pore type to the effective elastic properties by solving the elasticity problem for a pore of that type, and then incorporating the solution into a certain micromechanical method. For irregular pore shapes, the elasticity problem is usually solved numerically. However, actual microstructures may contain large numbers of diverse pore shape types, and solving elasticity problems for all of them with reasonable accuracy may become computationally challenging and practically impossible.

It is therefore desirable to be able to evaluate how irregularly shaped pores influence the effective material properties without having to solve the elasticity problem. For this purpose, researchers have been trying to identify the appropriate geometric parameters (in addition to the overall porosity of the material) to be used for the predictions of effective properties.

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Zimmerman (1991), for example, showed that compressibility of 2D pores correlates well with the undimensionalized ratio of pore perimeter Π to its area A defined as Π^2/A (a three-dimensional analog of this parameter, the surface-to-volume ratio, was used in the stochastic model of Drach et al., 2013). Zimmerman's observation was later supported by numerical studies on several irregular 2D shapes (Tsukrov and Novak, 2002). However, such a parameter cannot be considered universal. For example, substitution of smooth pore boundaries by the very jagged ones (as illustrated in Fig. 1) will significantly increase the surface-to-volume ratio without making big changes in the overall response. This immediately follows from the comparison (or "auxiliary") theorem of Hill (1965) as interpreted by Kachanov and Sevostianov (2005). According to their interpretation, contributions of two pores with very different surface-to-volume ratios shown by solid lines in Fig. 1 are bounded by the same contributions of pores shown with dashed lines. The influence of corrugated boundaries on the overall compressibility of pores is also discussed in Ekneligoda and Zimmerman (2008a).

Another possible set of geometric parameters to characterize contribution of a pore to the effective elastic properties is its principal moments of inertia (PMIs). PMIs are defined as the eigenvalues of the matrix of moments of inertia given by $I_{ij} = \int_V \rho(\mathbf{r})(r^2\delta_{ij} - x_i x_j)dV$, where $\rho(\mathbf{r})$ is the material density of the body for which PMIs are calculated (pores can be treated as homogeneous bodies with $\rho(\mathbf{r}) = \rho = 1$), r is the distance to the axis around which the moment is calculated, δ_{ij} is the Kronecker delta, x_i are the coordinates x_1, x_2, x_3. PMIs have been previously used to approximate pores by the equivalent ellipsoids (Li et al., 1999; Drach et al., 2013). In Drach et al. (2013) we utilized statistical approaches to correlate pore principal moments of inertia to their contribution to the effective elastic moduli.

In this paper we investigate the hypothesis that contribution of irregularly-shaped pores to the effective Young's moduli of porous material can be evaluated based on their projected areas ("shadows") by statistical analysis of effective compliance parameters. We begin by selecting a certain subset of pores from the full dataset. Then, we perform finite element (FE) simulations for the pores in the subset to quantify their individual contributions to the effective compliance of the material. This data is then used in regression analysis to construct an approximating polynomial model for the dependence of pore's contribution to the effective compliance on its projected area. To verify that the model works for the full dataset, the constructed model is then checked against the FE simulations on the new subset of randomly chosen irregular shapes not used in the model fitting.

Because the accuracy of the model predictions (width of the error bars) depends on the number of direct simulations used in the data fitting, it is important to choose an "optimal" subset which corresponds to the desired model prediction variance. We use the design of experiments (DoE) approach (Ryan, 2007; Myers et al., 2009) to identify the list of input parameters (in our case, pore shape geometric parameters) that corresponds to the specified level of model prediction variance across the whole parameter space. We design the "experiment" (the combination of irregular shapes for FE simulations) using an I-optimal design module in JMP software (SAS Institute Inc, 2010). The optimization criterion for I-optimal designs is minimization of the integrated variance of the model predictions over the entire design space. This means that the expected width of confidence intervals for model predictions will be approximately the same across the full parameter space.

We apply this method to two sets of pore shapes obtained by microcomputed tomography of two different material samples: carbon/carbon and 3D woven carbon/epoxy composites. The examples of pore shapes are given in Fig. 2. For both sets we compare contributions of the pores to effective elastic properties determined by the direct FEA simulations for each pore with the ones based on its projected areas. Note that we use these sets of pore shapes only to check the hypothesis that statistical estimates based on the projected areas can be used instead of elasticity solutions. Our predictions cannot be directly used for carbon/carbon and 3D woven carbon/epoxy composites, because in our analysis we assume the pores to be placed in an isotropic homogeneous material which is obviously not the case for these composites. However, we feel that the considered pore shape sets provide good data to test the hypothesis, as the pores in these two cases result from very different mechanical processes (porosity from incomplete filling by chemical vapor deposition of pyrolytic carbon vs. damage due to chemical and thermal shrinkage of epoxy) and thus have different morphologies and shape distributions.

2. Micromechanical modeling approach utilizing statistical analysis

Characterization of individual pore contributions to the effective material response is based on the pore compliance contribution tensor – $\mathbf{H}$ -tensor proposed in Kachanov et al. (1994). Note that a similar tensor in the context of a microcrack was earlier given by Horii and Nemat-Nasser (1983). The fourth rank tensor $\mathbf{H}$ 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 of a cavity:

$$\Delta\boldsymbol{\varepsilon} = \mathbf{H} : \boldsymbol{\sigma}_0 \quad (1)$$

where ":" denotes the contraction over two indices. For a material with a large number of pores, a proper representative volume element (RVE) (Hill, 1963; Nemat-Nasser and Hori, 1999) can be selected, and the effective compliance tensor of the material is given by

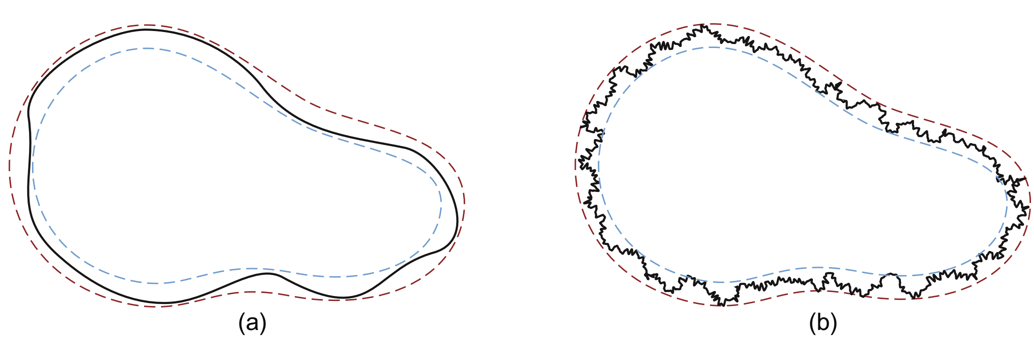

Fig. 1. Two pores having similar contributions to the overall elastic properties but significantly different surface-to-volume ratios. Dashed lines show upper and lower limits of their contributions.