DIGITAL-IMAGE-BASED STUDY OF CIRCULAR HOLES IN AN ELASTIC MATRIX

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ABSTRACT

Using a digital-image-based representation of a continuum composite, we apply computer simulation techniques to obtain the elastic moduli of a matrix containing randomly-centered circular voids. As the area fraction of the voids increases, the elastic moduli of the composite decrease until they eventually vanish at the percolation threshold. We compare our results with an effective medium theory, which predicts that Poisson ratio tends to a fixed value as the percolation threshold is approached, independent of the values of the elastic moduli in the pure system. Our results are also compared with recent experimental results.

INTRODUCTION

Calculating the elastic properties of a material that is made up of randomly distributed phases that have different elastic properties is a difficult problem that has received much attention [1]. Materials of interest range from semi-conductor alloys, where the random mixing of elastic properties is at atomic length scales, to fiber-reinforced materials, like SiC-whisker reinforced ceramics or steel-fiber-reinforced concrete, where the mixing occurs on macroscopic length scales. Atomic-scale composite problems are treated with lattice calculations, while macroscopic problems are usually treated with continuum mechanics.

This paper describes a merging of these two methods, using a new, simple finite-element-type scheme realized on a digital-image-based model of a two-dimensional two-phase material, where one of the phases has zero elastic moduli. This second phase is generated by punching out circular holes in a sheet. The holes are randomly-centered, so that they may freely overlap. The remaining area fraction of the matrix is denoted by \( p \). When the area fraction \((1-p)\) of circular holes reaches about 0.68, the holes percolate [2] and the elastic moduli of the sheet go to zero in a percolation transition.

DIGITAL-IMAGE-BASED MODEL

Representing images with pixels on a lattice is a technique that has been used for many years for quantitative image analysis [3]. Usually a square lattice of equal-sized square pixels is superimposed over an image, with the pixels being assigned to different phases of the picture according to whether or not the center of the pixel falls inside a phase boundary. Once the original continuum picture is thus represented digitally, all mathematical operations of interest can now be carried out on the underlying lattice, greatly simplifying their application.

The idea of breaking up a continuum into a lattice, and then carrying out mathematical operations on the lattice instead of the continuum is of course the basic idea behind finite-difference [4] and finite-element [5] methods for solving partial differential equations, and has been used for many years. The approach is to start out with continuum partial differential
equations, and convert them into linear algebraic equations by approximating derivatives by quotients of differences. This can of course be done for the partial differential equations of elasticity as well as any other set of equations.

In this paper we take a different approach. We represent a continuum model by pixels, and then use the underlying pixel lattice and material properties to define a random spring network having force constants that model the elastic properties of the original continuum material. Fig. 1 shows a portion of a 210 x 210 pixel triangular lattice of pixels, in which 11-pixel diameter circles have been introduced. The circles are all centered on pixels, so that their shapes are all exactly the same. The elastic network is defined by connecting nearest-neighbor pixels with the appropriate force constant spring, as will be discussed below. A space-filling triangular network of hexagonal pixels is used instead of a square network of square pixels, because the square lattice is unstable with only nearest-neighbor central-force springs [6,7].

![Image showing a 60 x 60 2-d triangular network of hexagonal pixels containing 4 randomly-centered 11-pixel diameter circular holes.](image)

**NUMERICAL METHOD**

Once an image is defined, as in Fig. 1, with a certain number of holes, a random spring network is created by connecting each pixel with its six nearest neighbors with springs of the appropriate force constant. Since the perfect triangular network with all the same nearest-neighbor springs obeys Cauchy’s relation, it is necessary to use more than one kind of spring in order to have a variable Poisson ratio [7]. Fig. 2 shows how three different kinds of springs, $\alpha$, $\beta$, and $\gamma$, are defined in the triangular spring lattice, so as to preserve isotropy, but allow for different values of Poisson ratio in the perfect lattice before any holes are introduced. For the perfect lattice, the area bulk modulus, $K_o$, and the shear modulus, $\mu_o$, are given by:

$$K_o = \frac{1}{\sqrt{12}} (\alpha + \beta + \gamma) \quad (1)$$
\[ \mu_o = \sqrt{\frac{27}{16}} \left( \frac{1}{\alpha} + \frac{1}{\beta} + \frac{1}{\gamma} \right)^{-1} \]  

The perfect lattice is isotropic because the \( \alpha, \beta, \gamma \) springs form three interlocking honeycomb lattices, which are elastically isotropic. In 2-d, the Young’s modulus \( E \) and area Poisson ratio \( \sigma \) can be found from the area bulk modulus and the shear modulus \( \mu \) through \[ E = \frac{4k\mu}{k + \mu} \]  

\[ \sigma = \frac{k - \mu}{k + \mu} \]

For the perfect lattice, using eqs. (1)-(4), the Young’s modulus \( E_o \) and Poisson ratio \( \sigma_o \) are given by:

\[ \sigma = 1 - \frac{2}{1 + \frac{2}{9} (\alpha + \beta + \gamma) \left( \frac{1}{\alpha} + \frac{1}{\beta} + \frac{1}{\gamma} \right)} \]

\[ E_o = \frac{2 \sqrt{3} (\alpha + \beta + \gamma)}{3 \left[ 1 + \frac{2}{9} (\alpha + \beta + \gamma) \left( \frac{1}{\alpha} + \frac{1}{\beta} + \frac{1}{\gamma} \right) \right]} \]

Fig. 2: Showing a piece of a triangular grid of hexagonal pixels. The three kinds of bonds, which connect centers of nearest-neighbor hexagonal pixels, have spring constants \( \alpha, \beta, \) and \( \gamma \).

Eq. (5) for \( \sigma_o \) allows values between 1/3 and 1 to be realized. It is convenient to use three, rather than two, parameters, because of the symmetry of the triangular network. The extra free parameter can be used as a consistency check.

When holes are introduced, springs with zero force constant are connected between pairs of
hole pixels and across the hole boundary, while $\alpha$, $\beta$, and $\gamma$ springs connect the matrix pixels.

Once the spring network has been set up, a uniaxial strain is applied, typically $-10^{-3}$. The nodes of the networks and the length of the unit cell perpendicular to the applied strain are simultaneously relaxed using a specialized conjugate gradient algorithm [9]. When the network is relaxed, the Young's modulus $E$ can be immediately obtained from the total elastic energy per unit area, and Poisson ratio $\sigma$ from the new length of the unit cell perpendicular to the applied strain. Equal tensile and compressive strains are used to average out any non-linearities, which were found to be small for strains $-10^{-3}$. Non-linearities are present because the (harmonic) springs in the network are not colinear.

EFFECTIVE MEDIUM THEORY

The problem of a single circular hole can be solved exactly, and this single-inclusion result forms the basis for effective medium theories (EMT). The simplest EMT for circular holes [9] in a 2-d sheet leads to the results:

$$\frac{E}{E_0} = 3p - 2 \quad (7)$$

$$\sigma - \frac{1}{3} = (\sigma_o - \frac{1}{3}) (3p - 2) \quad (8)$$

The other elastic constants can be obtained by inverting eqs. (3) and (4). The results (7) and (8) are remarkably simple, and are exact for small $(1-p)$, where it can be seen that $E/E_0$ is (unexpectedly) independent of $\sigma_o$. Indeed, eq. (7) predicts that $E/E_0$ is independent of $\sigma_o$ for all $p$. However, (7) and (8) incorrectly predict the percolation threshold $p_c$ to be $2/3$. In reality, percolation occurs $p_c \approx 0.32$ [2]. At percolation, the critical Poisson ratio reaches a universal value of $1/3$, independent of the Poisson ratio of the matrix material $\sigma_o$. Similar results have been found in lattice systems. The result can be understood by noting that any external stress will produce similar uniaxial strains in the narrow necks between adjacent circles at percolation.

The area fraction of material remaining, $p$, is related to the number of holes per unit area, $n$, via

$$p = e^{-na} \quad (9)$$

where $a$ is the area of a single circular hole. This is a statistical relationship that holds if a sufficiently large number of holes are present [10]. We have checked (9) in analysing our data, since $p$ may be evaluated directly by counting the number of matrix pixels remaining.

RESULTS

We have studied the dependence of the Young's modulus $E$ and the Poisson ratio $\sigma$ on $p$, the area fraction of the matrix material remaining, for three different choices of $\alpha$, $\beta$, and $\gamma$. These are $(\alpha, \beta, \gamma) = (1,1,1), (1,1,4), \text{ and } (1,6,7)$.

Two checks can be made on the accuracy of this digital-image approach. The first check is on whether we are really simulating a continuum system or not. The results for given values of
$E_o$ and $\sigma_o$ should not depend on the specific choice of lattice force constants, if we are truly carrying out a continuum simulation. Table I shows the results for $E/E_o$ and $\sigma$ at $p = 0.7377$, averaged over the same ten geometrical configurations. The first row is for $\alpha = \beta = 1$ and $\gamma = 4$, the second row interchanges $\alpha$ and $\gamma$, and the third row is for a completely different choice of force constants having the same values of $E_o$ and $\sigma_o$. The results on these three different systems all agree, to within less than 1%.

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$\beta$</th>
<th>$\gamma$</th>
<th>$E/E_o$</th>
<th>$\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>4</td>
<td>0.2899</td>
<td>0.3880</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>1</td>
<td>0.2898</td>
<td>0.3886</td>
</tr>
<tr>
<td>2</td>
<td>3.3</td>
<td>0.69</td>
<td>0.2916</td>
<td>0.3879</td>
</tr>
</tbody>
</table>

Table I: Continuum check on elastic moduli

The second check is on how accurately the single-hole exact result is reproduced. Eqs. (7) and (8) give the exact initial slope for the one-defect problem when $(1-p)$ is small:

$$\delta \sigma = \sigma - \sigma_o = (1 - 3 \sigma_o) (1 - p) \quad (10)$$

$$\delta E = \frac{E}{E_o} - 1 = -3 (1 - p) \quad (11)$$

Table II shows the percent difference from the exact result for $\delta E$ and $\delta \sigma$, for three different hole diameters $d$, and $(\alpha, \beta, \gamma) = (1, 1, 4)$. As expected, the results for $E/E_o$ become better as

<table>
<thead>
<tr>
<th>$(1-p)$</th>
<th>$d$</th>
<th>$\Delta(\delta E) %$</th>
<th>$\Delta(\delta \sigma) %$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00247</td>
<td>11</td>
<td>10.2</td>
<td>0.02</td>
</tr>
<tr>
<td>0.01077</td>
<td>23</td>
<td>3.2</td>
<td>0.03</td>
</tr>
<tr>
<td>0.02220</td>
<td>33</td>
<td>0.2</td>
<td>0.01</td>
</tr>
</tbody>
</table>

Table II: One-hole results

more pixels are used to define the circular hole. The diameter of 11 pixels used in this paper results in a 10% error in the change in $E$ caused by the introduction of one circular hole. The percent error in $E$ itself is, of course, very much smaller, less than a tenth of a percent. It is interesting to compare with the equivalent electrical problem. We have recently calculated the effect of one elliptical hole on the conductivity of a conducting sheet, using a square lattice digital-image scheme, and found that the error in the initial slope decreased linearly with the number of pixels used per unit length to represent the hole [11]. Table II implies that this error decreases more quickly for the elastic problem, as doubling the number of pixels per unit length caused the error to decrease by more than a factor of three, and tripling the number of pixels per unit length caused the error to decrease by more than a factor of 10. The surprising result in Table II is the fact that, at least for diameters greater than or equal to 11 pixels, the error in the initial slope for the Poisson ratio seems to be independent of the number of pixels per unit
length, and is essentially computer round-off error.

Figs. 3 and 4 present the results for $E/E_o$ and $\sigma$ vs. $p$, averaged over 10 configurations, and computed for the three choices of the force constants given above. The points are the simulation results, and the dashed lines are the effective medium results (7) and (8). The solid line is Fig. 3 is an interpolation-formula fit to the simulation data points, and is discussed below. In Fig. 3 it is interesting to note that it appears that $E/E_o$ is independent of $\sigma_o$ for all values of $p$, and not just for $p$ close to 1. We have independently computed $K/K_o$ and $\mu/\mu_o$, and have seen that they are clearly not independent of $\sigma_o$. Fig. 4 shows that $\sigma$ flows to a fixed point of about 1/3, as $p$ decreases, as was predicted by EMT. Interestingly, the flow to the fixed point is essentially complete by $p = 2/3$, the EMT percolation threshold, which is well above $p = 0.32$, the true percolation threshold [2]. The error bars on the Poisson ratio are large for $p \leq 0.6$. These are the statistical error bars from the 10 configuration average. The error bars of the Young’s modulus are much smaller as can be seen from Fig. 3. Although the Poisson ratio is computed directly, it can be regarded as the ratio of two elastic moduli, both of which become very small for $p \leq 0.6$. Nevertheless, the error bars in this region are disappointingly large.
For \( d = 11 \) pixel circles in a 210 by 210 lattice, we have directly computed the percolation threshold, using a lattice "burning algorithm" [12], and found it to be \( p_c = 0.34 \pm 0.03 \), in good agreement with the known result that was obtained using a true continuum simulation [2].

**SUMMARY**

We have shown that this simplest of finite element algorithms, a scheme based on linear Hookean springs, can give good results in 2-d composites. Such calculations are now feasible with the use of modern supercomputers. The calculations reported in this paper took ~ 150 hours of CPU time on a CYBER 205 supercomputer. It is important to emphasize that the present simple scheme, combined with averages over many samples to give good statistics, is best suited for the calculation of the elastic behavior of random composites. More sophisticated grids and algorithms have the capability of doing better on any particular realization, but that is not what is required here.

In the past, various EMTs have been compared with one another and checked against various exact bounds on the elastic constants [2]. This is rather unsatisfactory. The present work opens up the possibility of producing high quality numerical results on well-controlled composite geometries, in order to evaluate which, if any, EMTs are valid away from the dilute limit. A direct comparison between EMTs and real experiments is always dangerous because of the uncertainties present in the characterization of the geometry of real composites. Thus computer simulation can form an important bridge between approximate EMTs and experiments.

Recent experiments [13,14] have measured the elastic moduli of square sheets, containing randomly-centered circular holes, under uniaxial loading. Because of the clamping arrangement at the ends, a modulus intermediate between Young’s modulus \( E \) (completely free sides) and \( C_{11} = E/(1 - \sigma^2) \) (clamped sides). For simplicity, we compare our results for \( E/E_0 \) with the experiments in Fig. 5. This should be a good approximation, as our numerical results show that if \( \sigma_0 = 1/3 \), then \( \sigma = 1/3 \) for all \( p \). The materials used in the experiments [13,14] would be expected to have a Poisson ratio close to 1/3. To facilitate comparison between our simulations and the experiments, we have fitted our results to the empirical form

![Fig. 5](image_url)
\[ \frac{E}{E_o} = \left[ 1 - \frac{(1-p)}{m(1-p)} - \frac{m(1 - p_d) - (1 - p_d)}{m(1-p)(1-p)^2} \right]^m \] (12)

where we have set the initial slope parameter \(p_t = 2/3\); the percolation threshold \(p_c = 0.34\), to match our numerical results; and the exponent \(m = 3.4\) is obtained by a least-squares-fit to the simulation data. The experimental data points have been obtained from the published graphs using image analysis.

The exponent \(m\) is not meant to be a critical exponent, as our data is quite far from the critical region near \(p_c\). Rather, \(m\) is merely a free parameter in the interpolation formula (12). It is very difficult to obtain good results in the critical region as \(E/E_o\) is so small. On theoretical grounds, the true critical exponent \(f\) is expected to be about 5.1 [13-15].

The interpolation formula (12) fits the data in Fig. 3 well. Fig. 5 shows that the interpolation formula, with the same exponent \(m\), also fits the data from Ref. 13. For reasons that are not clear to us, the data from Ref. 14 is systematically quite far above our results.

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REFERENCES

[9] This algorithm was written by and can be obtained from A.R. Day, at the address given above.