FINITE ELEMENT ANALYSIS OF POROSITY ON MATERIAL PROPERTIES USING MSC/NASTRAN

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Abstract

In this paper, a finite element model using MSC/NASTRAN is developed that can numerically determine the material's modulus of elasticity using the limited information from one material sample. The model is three dimensional, and simulates pores by placing small elements that are non-load bearing into the structure. These voids are randomly and unevenly distributed (using a Poisson distribution) to better simulate the response of a real porous material to a load. The porous model deformation can be used directly to calculate the porous modulus of elasticity. The model is shown to be accurate.

The same finite element model is used to demonstrate the effects on material behavior of changing the pore size and distribution. From this information a trend was noticed and an empirical equation developed that predicts a material's elastic modulus based on porosity and pore size.

Introduction

Porosity exists in almost all materials to some extent. Therefore the effects of porosity should be of concern to any material developed for a design. Porosity is of particular interest to a designer who plans to use ceramic materials, because it is unavoidable in ceramics. Sometimes porosity is desirable for other than structural reasons such as heat transfer properties, easier production (bringing lower cost), radar reflection, etc.

When dealing with porous materials, there are two structurally oriented concerns: (1) the onset of a pore growing into a crack, and (2) the macroscopic effects of the pores on material strength. This paper is concerned primarily with the macroscopic effects of porosity. The growth of pores into cracks will be discussed only briefly for completeness. The modulus of elasticity, also called Young's modulus, is the major parameter of interest when looking for the macroscopic effects of porosity.

This paper is an attempt to create a finite element model that simulates a porous material. With this finite element model the porosity, pore size, and distribution can be varied to see the effects on the overall material. The finite element model uses a common "off the shelf" computer code, MSC/NASTRAN. The computer model used in this thesis only used linear elastic deformations, but it can be extended into the nonlinear regime. Even though plastic deformation and microcracking are significant effects on the microstructure, it will be apparent that a reasonably accurate model of the macroscopic effects of porosity can be made using only linear elastic calculations.

Background

Porosity is defined as the fraction of volume occupied by non load carrying voids in the material. Past work on the effects of porosity on Young's modulus has primarily dealt with fitting an empirical curve to actual data for a specific material. Thus for every material one had to make dozens of samples, each with different porosities, and then try and fit a curve to the data points to show how Young's modulus varied with porosity. Three equations in particular have been extensively used to curve fit the data [Ref 1 & 2]. They are the linear equation (1), the exponential equation (2), and the semi-empirical equation (3) (which was originally deduced by Hasselman [Ref 3] from work done by Hashin [Ref 4]);

$$E = E_o(1 - \alpha P) \tag{1}$$

$$E = E_o e^{-bP} \tag{2}$$

$$E = E_o \left[1 - \frac{AP}{1 + (A - 1)P} \right] \tag{3}$$

where

E = Elastic modulus (Young's modulus)
E_o = Elastic modulus without any porosity, found empirically
A = an empirical constant
P = volume porosity
α = slope, an empirical constant
b = an empirical constant

While the curve fitting method has proven to be reasonably accurate, it is also time consuming, and requires extensive lab work. Also, there was no way for a material engineer to predict the results of changing an untested material's porosity without actually producing the material and testing it. Furthermore, previous work did not adequately predict the

effects of changing the pore sizes, or pore distribution. This paper tries to rectify that condition.

Model Creation

The first step in coming up with a predictor was to create a finite element model that simulated the microstructure of a porous material. Previous finite element models of porous materials [Ref 5 & 6], used two dimensional circular voids evenly spaced in a material. Instead, a three dimensional model, with cubic voids, in a random and uneven distribution was chosen for this analysis. Also, unlike previous works, linear elastic deformation was chosen for this analysis. Cracking and plastic deformation were not considered. Fortunately the model selected, after some refinement, did a good job of predicting the properties of the studied materials.

After some small scale finite element testing, it was determined that for MSC/NASTRAN an 8-noded CHEXA element gave the most accurate results. The 20-noded cubical elements were too stiff.

The overall model used was a block, and the size varied with each test case. This block was divided into 80 cubes called cells. The block had dimensions of four cells by five cells. More cells were put in the Z direction, as that was the direction force would be applied. The force applied to the top plane of the model.

Each cell was then made by an image superelement of one of the primary superelements. The primary superelements were a collection of elements simulating zero, one, two, or more pores inside of a cell. Figure 1 shows the overall model with only the primary superelements shown. Figures 2, 3, and 4 show the cells with one, two, and multiple pores, respectively.

Unlike previous models which assumed all pores to be round, this model assumed all pores to be cubes. This was done primarily to simplify the model. However, Figure 5 shows a picture of a porous material (cobalt oxide) and it is evident that the pores (black areas) are irregular angular shapes situated between grain boundaries. Therefore an argument can be made that pores are more accurately (or at least as accurately) simulated by cubes rather than by spheres.

This model makes extensive use of superelements to greatly reduce processing time. Image superelements are supèrelements that are repeated several times in the model. This reduces calculations because once the primary superelement has been solved, each of the image superelements can use the same stiffness matrix.

Now that cells with different number of pores in them can be simulated, how should the model be populated? First an even

distribution of one pore per cell was tried based on a paper by R.D. Thomson and J.W. Hancock [Ref 7] which discussed the effects on non-homogeneous void distributions. In the case of a cell with x inclusions in it, Thomson and Hancock used the following Poisson distribution equation:

$$P(x) = \frac{\bar{x}^{(x-1)}}{e^{\bar{x}}(x-1)!} \qquad (4)$$

where

P(x) = probability of there being x pores in the cell
x = number of inclusions in the cell
e = the Napier number, 2.71828...
$\bar{x}$ = average number of pores per cell

The average number of inclusions per cell is then obtained from:

$$x = \frac{V_{\bar{x}}}{V_1} \qquad (5)$$

where

$\bar{x}$ = average number of pores per cell
$V_{\bar{x}}$= average number of pores per cell
V_1 = volume of average cell with one pore
The volume of the average cell with one pore is:

$$V_1 = \frac{V_P}{P} \qquad (6)$$

where

V_1 = volume of average cell with one pore
V_P = pore volume
P = volume porosity

Therefore, using known information; pore size, cell size, and volume porosity; Equations 4,5, and 6 can be used to calculate the probability of a cell having x number of pores. Once the probability distribution is known, it is a simple matter to allocate a certain number of cells in the 80 cell model to match the probability distribution.

Equation 10, below, was used to turn the MSC/NASTRAN output into a modulus of elasticity data point. Equation 10 was derived using the linear stress-strain relationship (Eqn. 7), the definition for one dimensional stress (Eqn. 8), and the definition for one dimensional strain (Eqn. 9).

$$\sigma = E\varepsilon \tag{7}$$

$$\sigma = \frac{F}{A} \tag{8}$$

$$\varepsilon = \frac{\Delta Z}{L} \tag{9}$$

$$E = \frac{FL}{A\Delta Z} \tag{10}$$

where

E = calculated modulus of elasticity
F = total applied upward force to the top of the model
A = model top end area
ΔZ = displacement of the top of the model
L = model height

Equation 10 was used throughout all of the testing to calculate what the total model's modulus of elasticity was for that test. For the distributed pore cases, since the cells were distributed randomly, the final displacements on the top end of the model are uneven and average displacements were used.

Results

Cobalt Oxide

If the porous material computer model was going to be useful, the predicted results had to match laboratory tests for an actual material. The material initially chosen was cobalt oxide (CoO) because of the wealth of information known about it. From the grain structure one can measure the average pore size to be about 8 micrometers (i.e. 8×10^{6} meters). This average ignores places where two pores have combined into one, since the model takes into account multiple pores that touch each other.

First, evenly distributing the pores, one per cell, was tried. For this case the total porosity was changed by changing the pore size. The results are shown of Figure 6 (the symmetric distribution). Comparing the results of this case to the actual test data, also shown on Figure 6, one can see that evenly distributing the pores causes the modulus of elasticity to be much higher, and drop much slower as porosity increases, than the real test values.

Next a Poisson Distribution was tried. This put more pores in some cells and fewer in others, while keeping the pore size of 8 micrometers constant. Figure 6 shows that the slope using distributed pores is much steeper than the case for evenly distributed pores (i.e. modulus of elasticity for this case drops much faster as porosity increases). In fact, the slope is close to the actual test results once they are linearly curve fitted, but for some reason all the computer model values are high. This is unusual since the value of zero porosity Young's modulus (E_o) used for the solid elements is the same as the linear approximations intercept point for zero porosity (E_o = 29.3 x 10^6 psia). Thus, one would expect the interception with zero porosity to be about the same, and all the values to be close to the same since the slope is close.

To correct this problem, the value for the modulus of elasticity of the solid elements was dropped to 26.1 x 10^6 psia. The results are close to the actual data.

Silicon Carbide

Next a demonstration that the model worked for other materials was needed. The material used next was silicon carbide (SiC). Ruh (Ref. 9) states that silicon carbide has a reasonably consistent average grain sizes of 2.5 micrometers (2.5 x 10^{-6} meters), and gives a value of zero porosity elastic modulus (E_o = 440 Giga Pascals) as the linear equations zero porosity intercept point. Figure 7 shows the results of using this data in the computer model. This first run was slightly high just like the first cobalt oxide case, but lowering the value of zero porosity elastic modulus (E_o) to 425 Giga Pascals gives results that almost exactly matches the actual test data.

This demonstrates that the model was accurate for more than one material. It also shows that the value of zero porosity elastic modulus used in the computer model should be about 5% lower than the linear equation would predict it to be.

Aluminum Nitride.

It has always been difficult to get a close correlation between porosity and elastic modulus for minimum nitride because aluminum nitride pores vary greatly in size and shape depending upon the manufacturing techniques. Table 1, from Ruh [Ref 9], shows how much pore size can vary. Notice that larger pore sizes seem to cause a much larger elastic modulus even if the porosity is about the same. For example: sample 6 has a larger porosity than sample 5 and larger (not smaller as would normally be expected) elastic modulus due to much larger pore sizes.

Sample no.	Origin *	Porosity (%)	Pore size micro m	Elastic Modulus million psia
1	STK/-400/1700/5	0.5	2-10 (5)	46.6
2	Fabricated by GE	1.7	1-3	44.5
3	AT/ar/1700/30	4.1	1-20 (10)	40.8
4	AT/ar/1700/40	4.7	1-20 (10)	42.3
5	STK/ar/1700/30	5.4	2-8	38.6
6	AT/ar/2100/60	5.6	5-50 (10)	42.1
7	AT/ar/1750/15	6.0	1-5	37.9
8	STK/ar/1700/20	10.5	2-6	34.9
9	AT/ar/1850/30	12.9	2-10 (5)	34.0
10	AT/+400/1600/15	13.2	5-120	36.5
11	AT/+400/1700/15	14.0	5-120	36.4
12	STK/ar/1600/30	16.1	1-10 (5)	34.3
13	AT/ar/1950/30	18.4	2-20 (10)	29.7
14	STK/ar/1600/30	21.2	2-20 (10)	27.8
15	AT/+400/1700/20	23.9	3-250	23.4

* = Starting powder/ Particle size/ Hot-pressing temp (°C)/ Time (min)
STK = Stack, AT = Atommergic, ar = as received, GE = General Electric

Table 1. Microstructure Data for Aluminum Nitride

Aluminum nitride was modeled next to find out how pore size affected the microscopic material behavior, and if the computer model simulated this change properly. First, cubic pores with each side 8 micrometers long were tested. Figure 8 shows that the results fit quite close to the actual test data given.

Next, five micrometer pores were tested. The results were much too high elastic modulus for porosities above two or three percent. The reason for this was that the cell size was too big for the smaller pore size. To get large porosities, i.e. above 5 percent, large conglomerations of up to ten pores in one cell were needed, and few, if any, cells with only few pores in them were used. Essentially this means that the model was really modeling larger pores, one per cell, not small scattered pores.

This was solved by making the cell smaller, 12 micrometers instead of 20 micrometers. This made distributions of zero, one, and two pore cells much more prevalent, and eliminated eight, nine, and ten pore cells. The results, shown in Figure 8, were reasonably close to the actual data point for five micrometer pores, shown if Figure 8 by an asterisk. Figure 8 also shows that the 5 micrometer pore results are almost identical to the 8 micrometer pore results.

If the ten micrometer pore results were not significantly different from the 5 and 8 micrometer pores, then the model may not have been properly accounting for pore size. The 10 micrometer pore tests shown in Figure 8 were in fact higher than the 5 and 8 micrometer pore results. They were also quite

close to the actual test results, as shown in Figure 8. The 10 micrometer tests showed that the model did, therefore, show the effects of increasing pore size, i.e. as pore size grows the elastic modulus decreases slower as porosity increases.

Lastly, 15 micrometer pores were tried to see if the trend continued. Figure 8 shows that the trend not only continues, but increases. In other words; as the pore size increases the negative slope of the elastic modulus versus porosity line decreases at a faster and faster rate. This would explain why there was very little difference between the 5 and 8 micrometer pore results.

Derived Equation

From the aluminum nitride model, a trend can be seen relating the pore size with the rate of change of elastic modulus to porosity. Therefore, the next task is to try and find an equation that describes this trend. This was done by taking the computer generated data and trying to fit it to the previously used equations; linear (Equation 1), empirical exponential (Equation 2), semi-empirical (Equation 3), and empirical power (Equation 7). It was found that the linear Equation 1 gave the most consistently reasonable fit. Using the linear Equation 1 means that only the parameter for the slope, a, needs to be modified for the various pore sizes.

Table 2 shows all the data correlating slopes to pore size, for the cases studied in this paper.

Pore Size Micro m.	Slope	Material
2	2.103	Si C, actual test data
5	2.157	Al N, actual test data
5	2.247	Al N, computer data
8	2.720	Co O, actual test data
8	2.201	Al N, computer data
10	2.048	Al N, computer data
10	1.908	Al N, actual test data
15	1.351	Al N, computer data

Table 2. Slopes for Various Pore Sizes

The Shareware program CURVEFIT [Ref 10] was used to find an equation that best describes how slope, a, changes with pore size. The result is again the Cauchy distribution equation;

$$\alpha = \frac{1}{P1(L + P2)^2 + P3} \qquad (11)$$

where

a = parameter, slope, for Equation 1
L = pore size (length, diameter, etc.) in micrometers
P1= a constant, in this case 0.003866
P2= a constant, in this case -5.988
P3= a constant, in this case 0.4275

Figure 9 shows how Equation 11 is only an approximation to the actual data given in Table 2. Putting the results from Equation 11 into Equation 1 gives:

$$E = E_o\left(1 - \frac{1}{P1(L + P2)^2 + P3} P \right) \qquad (12)$$

where

E = Elastic modulus (Young's modulus)
E_o= Elastic modulus without any porosity
L = pore size (length, diameter, etc.) in micrometers
P1= a constant, in this case 0.003866
P2= a constant, in this case -5.988
P3= a constant, in this case 0.4275
P = volume fraction porosity

Applying Equation 12 to the cases that have been looked at in this paper (i.e. cobalt oxide, silicon carbide, and aluminum nitride) give very accurate results, shown in Figures 10, 11, and 12, respectively. While Equation 12, which estimates elastic modulus based on pore size and porosity is not perfect, it is close enough to give a material designer a good starting estimate of how a new material would behave.

To verify Equation 12, it should be used for some test case. Information on the pore size of materials is scarce, so aluminum nitride will be used again, but this time for different pore sizes not previously examined. Referring back to Table 1, data point 2 has 1.7% porosity, 2 micrometer pores (average) and the same zero porosity elastic modulus for aluminum nitride is about 46.7 million psia. Putting this data into Equation 24 gives an elastic modulus of 45.07 million psia. Putting this data into Equation 24 gives an elastic modulus of 45.07 million psia, where the actual tested number is 44.5 million psia. This is only 1.28 percent error, extremely good for an empirical first approximation. Several

other data points from Table 1 were tested, and Table 3 below shows the results. In all cases the error was small, but usually not ignorable.

Sample (Table 1)	Porosity (%)	Pore size micro m	E (tested) million psia	E (calculated) million psia	Error (%)
2	1.7	2.0	44.5	45.07	1.28
5	5.4	4.0	38.6	41.00	6.22
7	6.0	2.5	37.9	40.79	7.62
8	10.5	3.0	34.9	36.08	3.38
10	13.2	12.0	36.5	35.80	1.92
11	14.0	12.0	36.4	35.1	3.57

Table 3. Verification for Aluminum Nitride

Conclusions

Up until now a material designer had to actually make and test several samples of a material, and curve fit the results to one of several empirical formulas (linear, exponential empirical, semi-empirical) to see how a material behaved as porosity changed. This paper has presented an alternative to actual production and testing.

For materials that are linearly elastic, like most ceramics, with average pore sizes between about 1 and 20 micrometers, one could get an initial estimate by using Equation 12. This equation gives valuable information showing how pore size and porosity effect the materials elastic modulus.

A closer prediction of actual material behavior can be obtained through the application of the finite element model. This computer model gave accurate results, with only slight error when compared to lab test results, for all materials analyzed. This finite element model can also be applied to materials that are not linear elastic using other MSC/NASTRAN solution algorithms, if the stress-strain curve for the zero porosity material is known.

In summary, the strength of a porous material depends primarily on volumetric porosity, and pore size. This thesis has developed an equation and a computer model which can be used to predict a material's elastic modulus using only pore size, porosity, and zero porosity elastic modulus.

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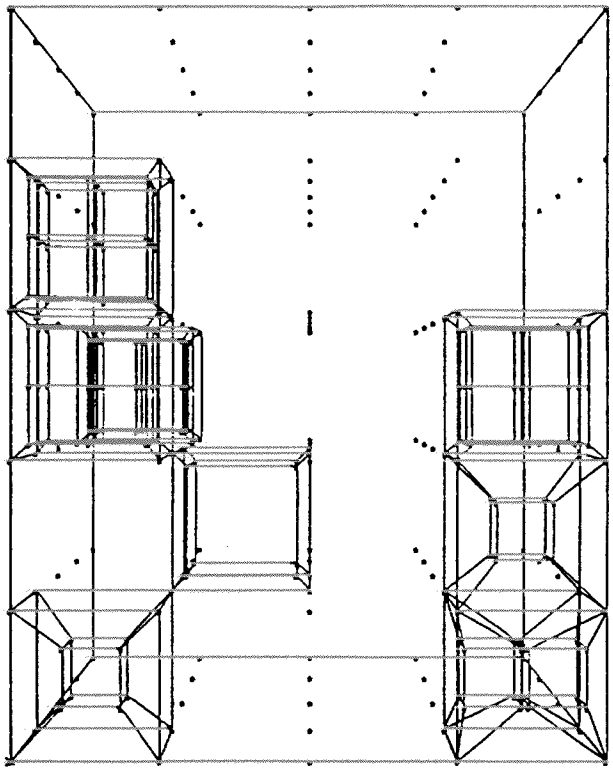

Figure 1. Final Computer Model

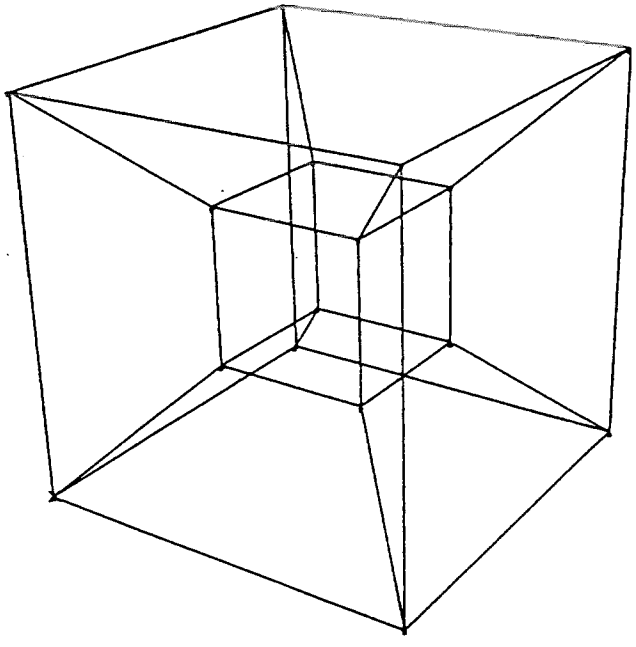

Figure 2. Single-Pore Cell

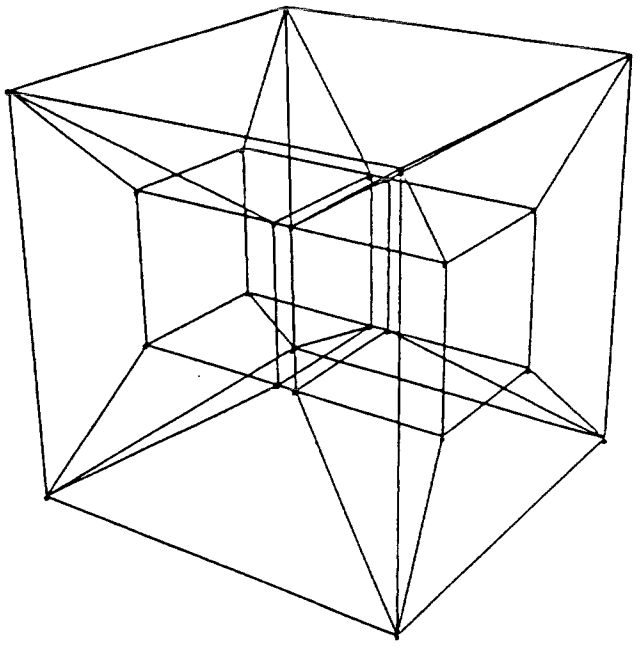

Figure 3. Double-Pore Cell

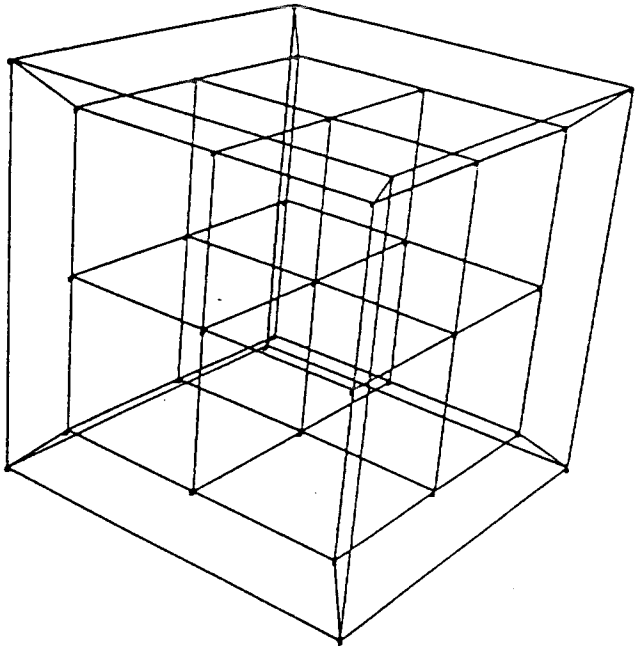

Figure 4. Cell With Three to Eight Pores

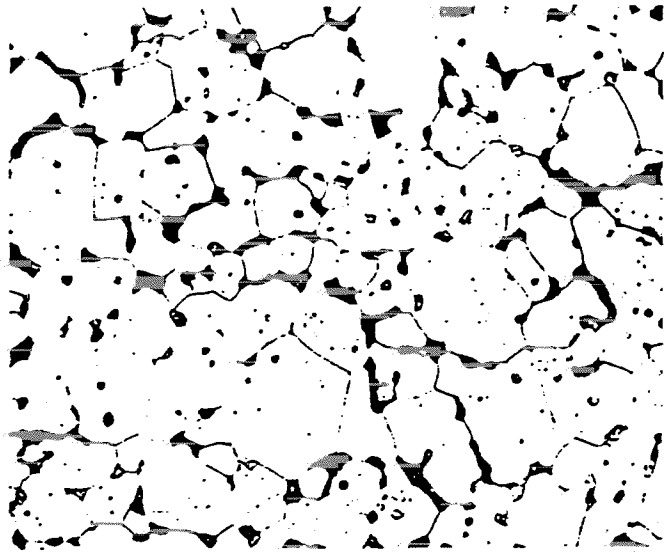

Figure 5. Cobolt Oxide, x400 Magnification

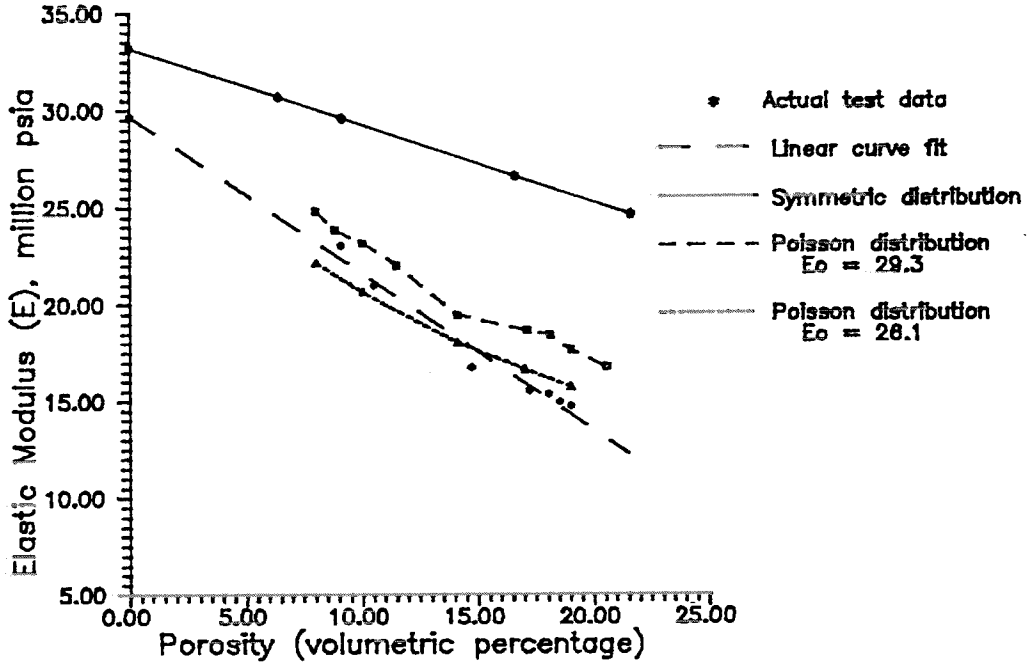

Figure 6. Cobolt Oxide Elastic Modulus vs Porosity

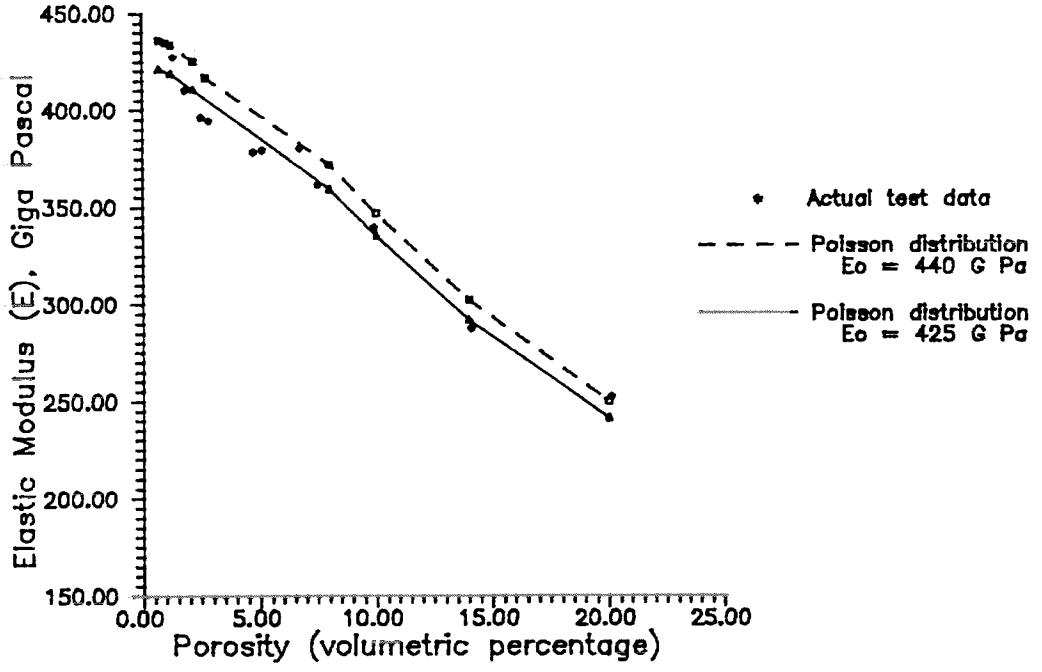

Figure 7. Silicon Carbide Elastic Modulus vs Porosity

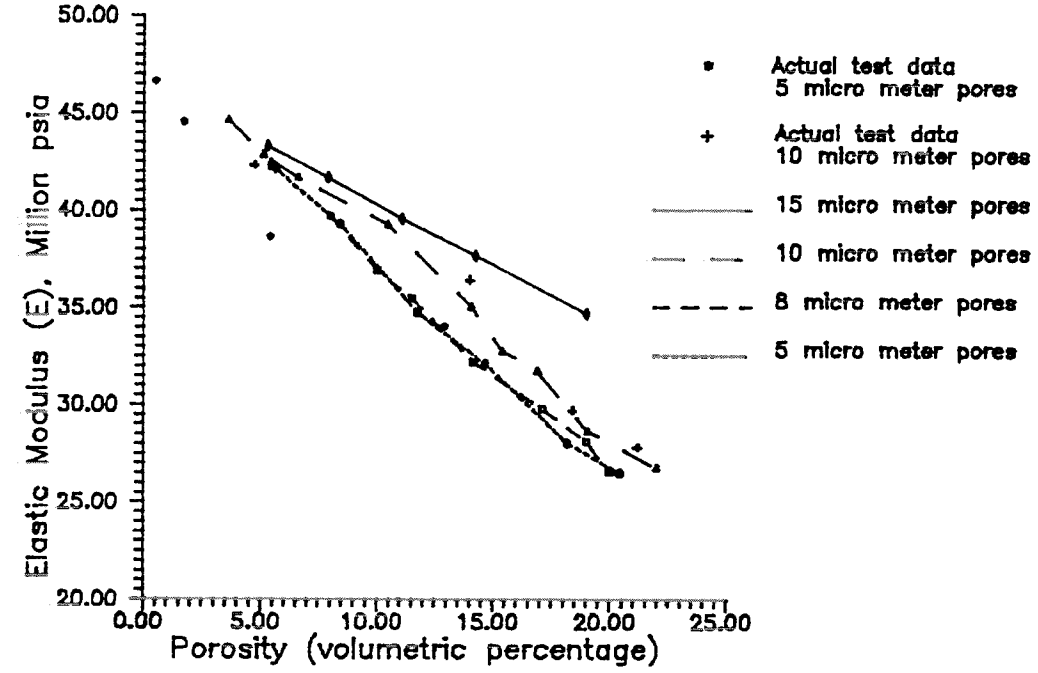

Figure 8. Aluminum Ntride Elastic Modulus vs Porosity

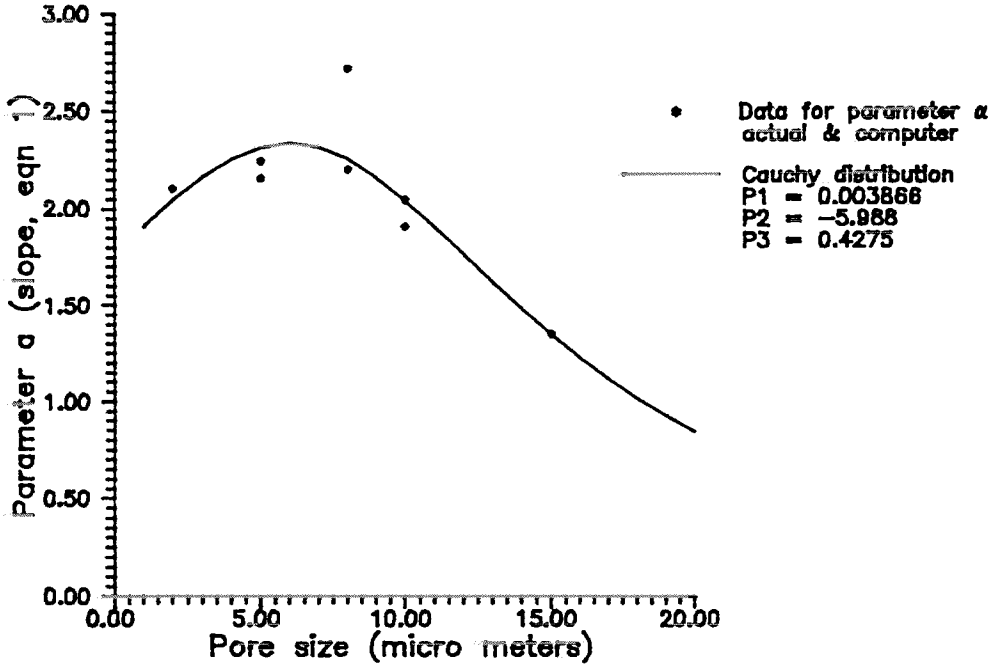

Figure 9. Relationship Between Parameter α and Pore Size

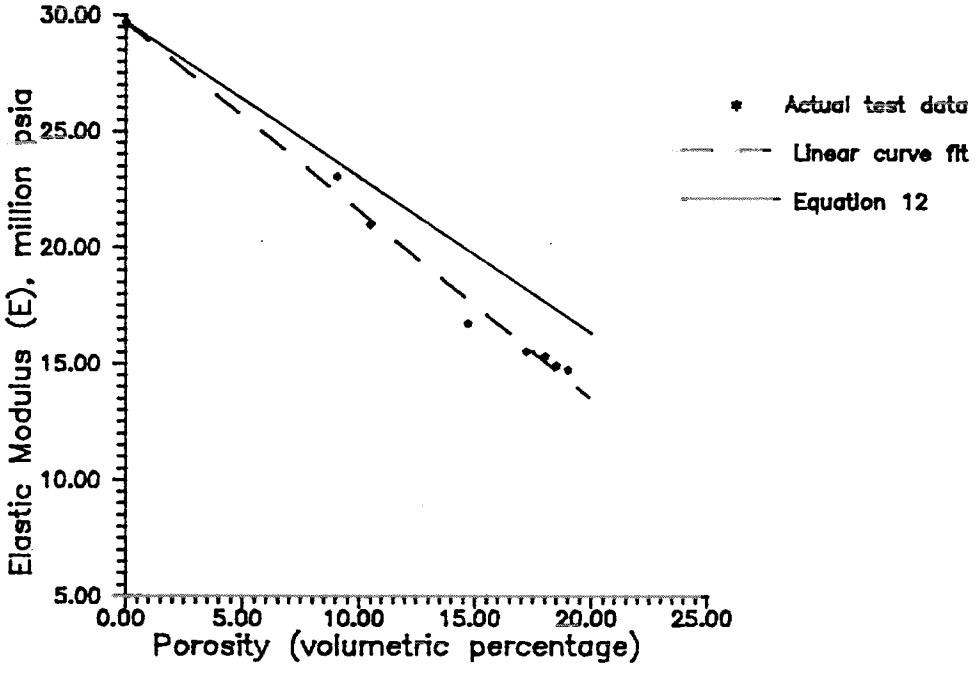

Figure 10. Cobolt Oxide Elastic Modulus vs Porosity

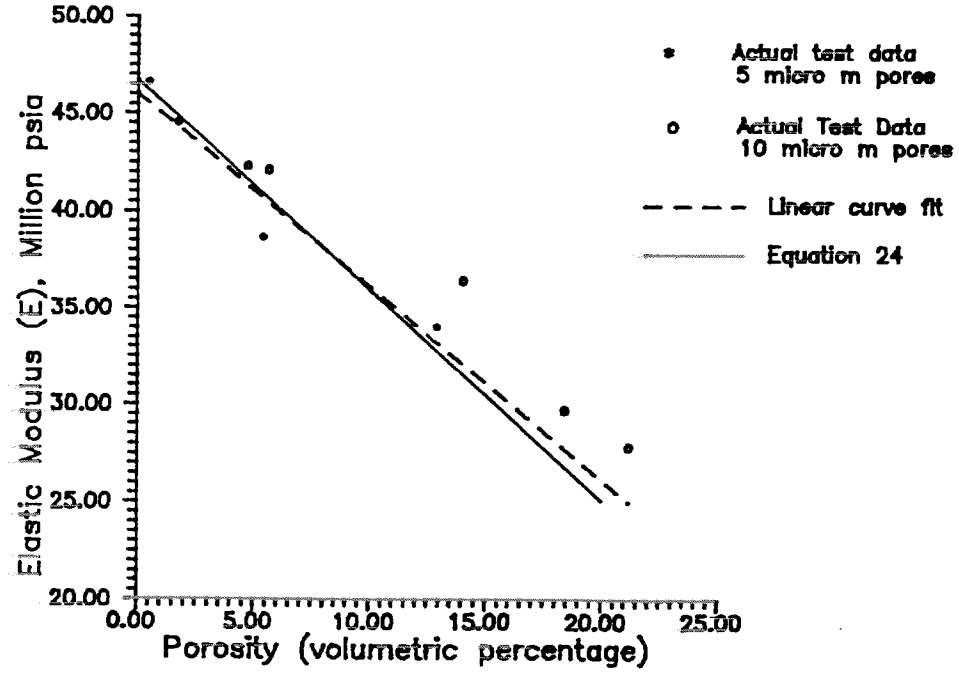

Figure 11. Silicon Carbide Elastic Modulus vs Porosity

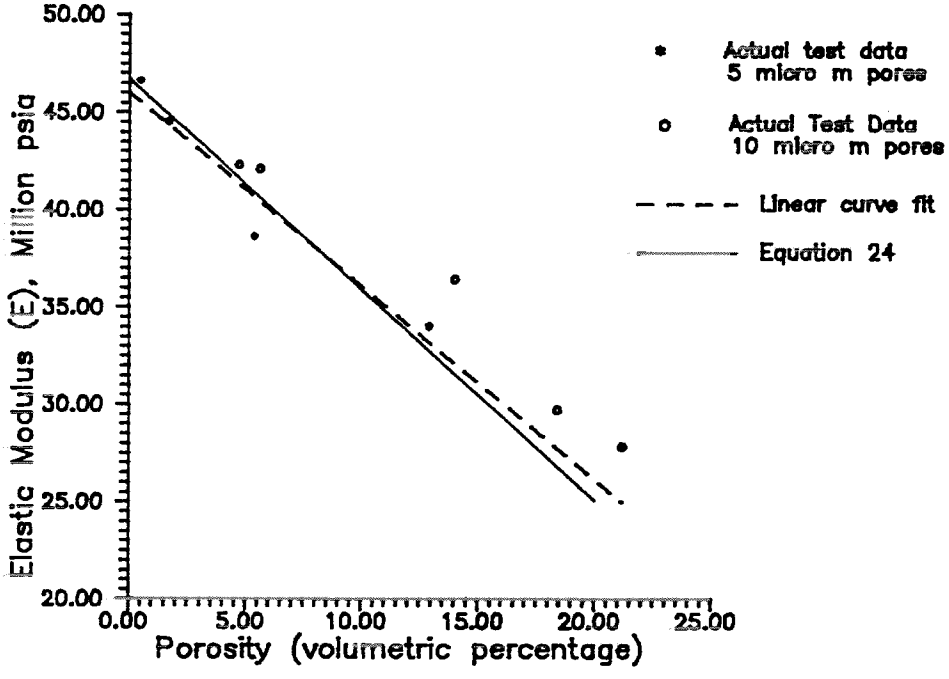

Figure 12. Aluminum Nitride Elastic Modulus vs Porosity