Crystal Elasticity using FFT

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1 Introduction

In this assignment we will try to model elasticity of materials with different zener ratios and also try to model the stress and strain field in a plate with a hole in it.

2 Different Zener Ratios

An artificial microstructure was generated using Dream3D. This was then subjected to a strain and the material's response was calculated with a code which uses FFT technique. The material's response was calculated for various zener ratios and then a histogram of equivalent stress normalized with respect to its average equivalent stress was plotted. A code in MATLAB was written to calculate the normalised equivalent stress and plot the histogram and box plots.

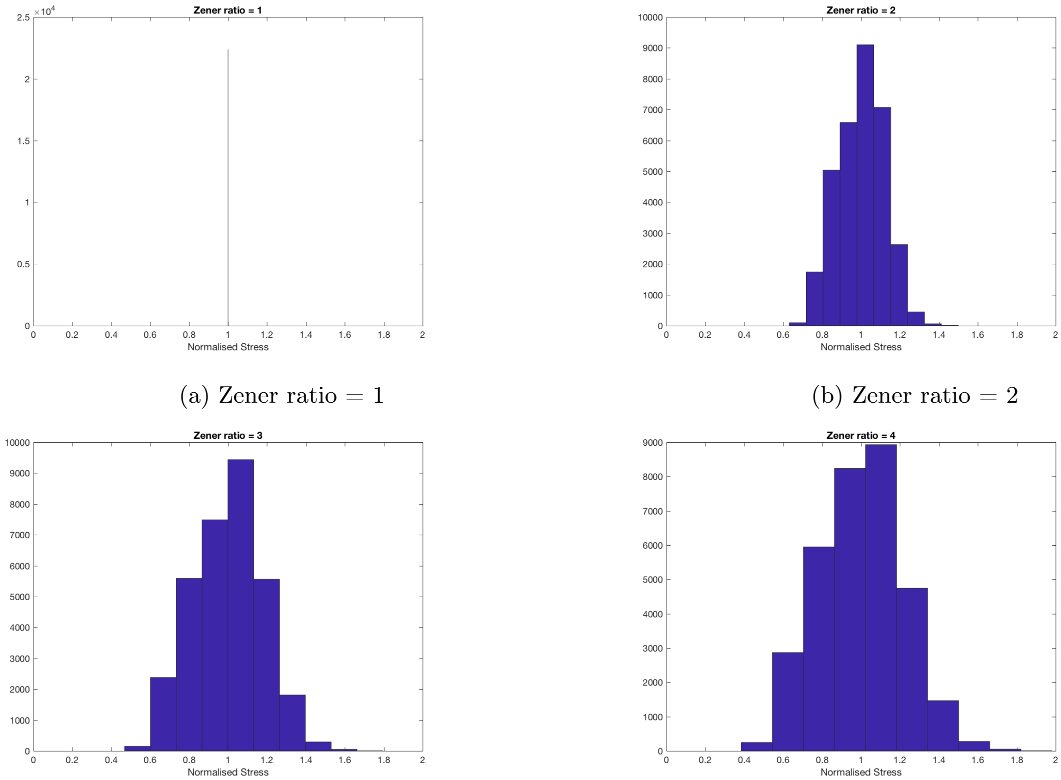
```
%% To calculate equivalent stress
 for i = 1:len
     temp = (SLOC1(i) - SLOC2(i))^2 + (SLOC2(i) - SLOC3(i))^2 + (SLOC3(i) - SLOC1(i))^2;
     temp = temp + 6*((SLOC4(i))^2+(SLOC5(i))^2+(SLOC6(i))^2);
     eq_stress(i) = sqrt(temp/2);


 end

 avg_stress = sum(eq_stress)/len;

% Normalising the eqivalent stress
 for i = 1:len
     eq_stress(i) = eq_stress(i)/avg_stress;
 end


%% To plot the histogram
hist(eq_stress_1)
xlim ([0 2])
xlabel('Normalised Stress');
title ('Zener ratio = 1')
str1 = ['zener1'];
print(str1,'-dpng');
```

The stiffness properties given as input to the above code is given in 1. The properties are in GPa.

C_{11}	C_{12}	C_{44}	Zener ratio
1.700	1.240	0.230	1
1.700	1.240	0.460	2
1.700	1.240	0.690	3
1.700	1.240	0.920	4

Table 1: Stiffness Properties used for calculations

A bar plot is made for the normalised equivalent stress as shown in fig 2



(a) Zener ratio = 1

(b) Zener ratio = 2

(c) Zener ratio = 3

(d) Zener ratio = 4

Figure 1: Histogram of normalised Equivalent stress for different zener ratios

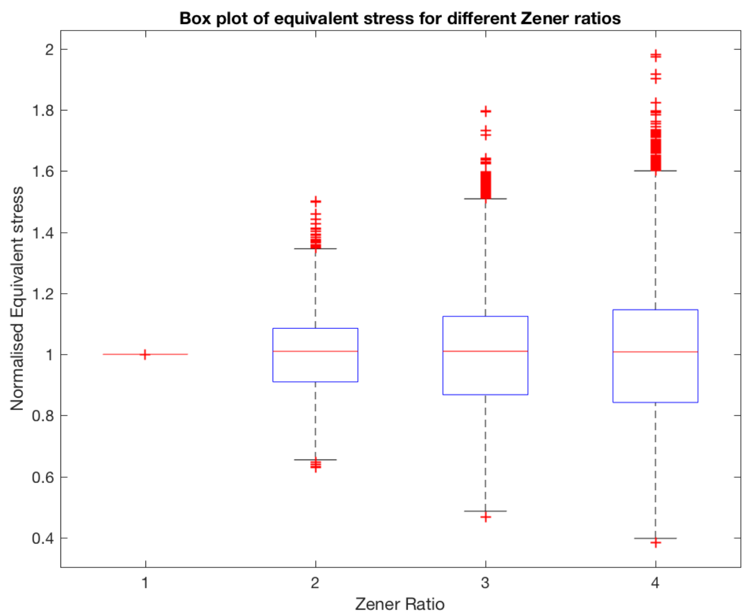
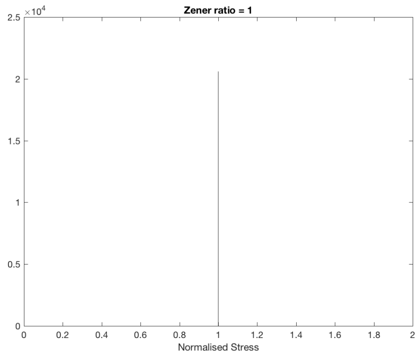
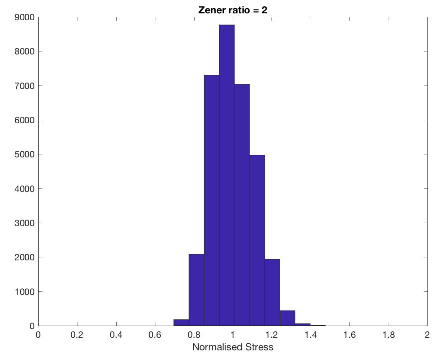


Figure 2: Box plot normalised Equivalent stress for different zener ratios

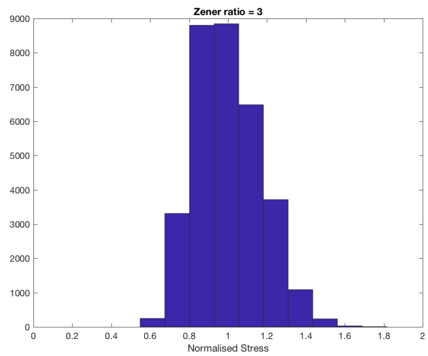
A similar code was run to plot the normalised equivalent strain.



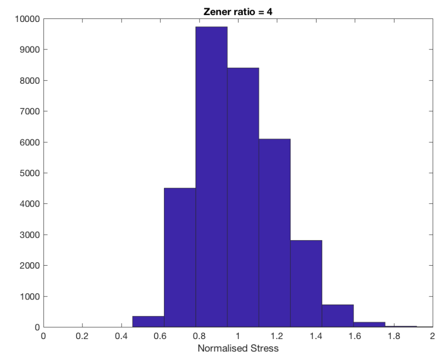
(a) Zener ratio = 1



(b) Zener ratio = 2



(c) Zener ratio = 3



(d) Zener ratio = 4

Figure 3: Histogram of normalised Equivalent strain for different zener ratios

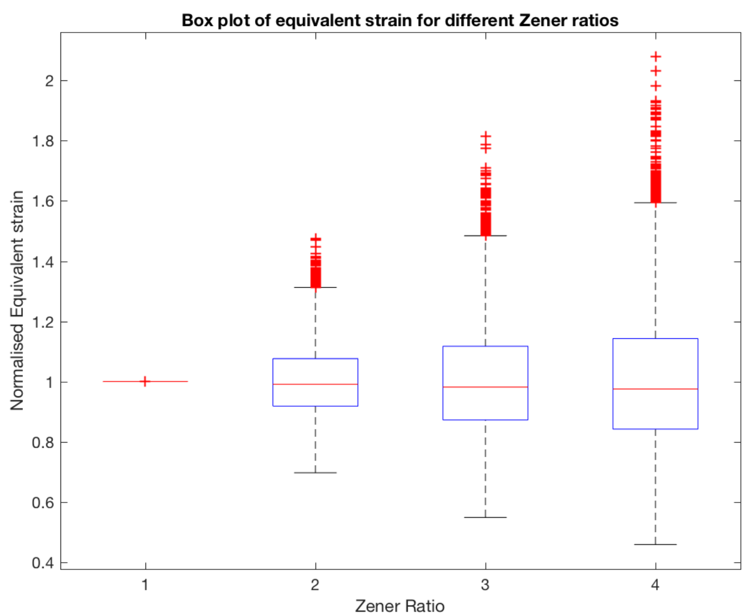


Figure 4: Box plot of normalised Equivalent strain for different zener ratios

3 Hole in a plate

A code was writen to generate a plate with a hole in between.The MATLAB cod to genreate the microstructute is given below.The microstructure generated is as shown in fig 5. This was then given as the input for the FFT code and the stress field was calculated.

```
%% Dimensions of the domain and hole
Nx = 128;
Ny = 128;
num = Nx*Ny;
matrix = zeros(Nx*Ny*2,8);
rad = 5;
%% Generate the microstructure
for i = 1:Nx
    for j = 1:Ny
        k = (j-1)*Nx + i;
        dist = (i-Nx/2)^2 + (j-Ny/2)^2;
        % For generation of a hole
        if(dist<rad*rad)
            matrix(k,1) = 0.0;
            matrix(k,2) = 0.0;
            matrix(k,3) = 0.0;
            matrix(k,4) = i;
            matrix(k,5) = j;
            matrix(k,6) = 1;
            matrix(k,7) = 2;
            matrix(k,8) = 2;
            matrix(k+num,1) = 0.0;
            matrix(k+num,2) = 0.0;
            matrix(k+num,3) = 0.0;
            matrix(k+num,4) = i;
            matrix(k+num,5) = j;
            matrix(k+num,6) = 2;
            matrix(k+num,7) = 2;
            matrix(k+num,8) = 2;
        % For generation of parent hole
        else
            matrix(k,1) = 90.0;
            matrix(k,2) = 90.0;
            matrix(k,3) = 90.0;
            matrix(k,4) = i;
            matrix(k,5) = j;
            matrix(k,6) = 1;
            matrix(k,7) = 1;
            matrix(k,8) = 1;
            matrix(k+num,1) = 90.0;
            matrix(k+num,2) = 90.0;
            matrix(k+num,3) = 90.0;
            matrix(k+num,4) = i;
            matrix(k+num,5) = j;
            matrix(k+num,6) = 2;
            matrix(k+num,7) = 1;
            matrix(k+num,8) = 1;
        end
    end
end
%% Write it to a file
dlmwrite("text.txt",matrix,'delimiter','\t');
```

The stress field calculated is plotted along a line from the edge of the hole to edge of the material.

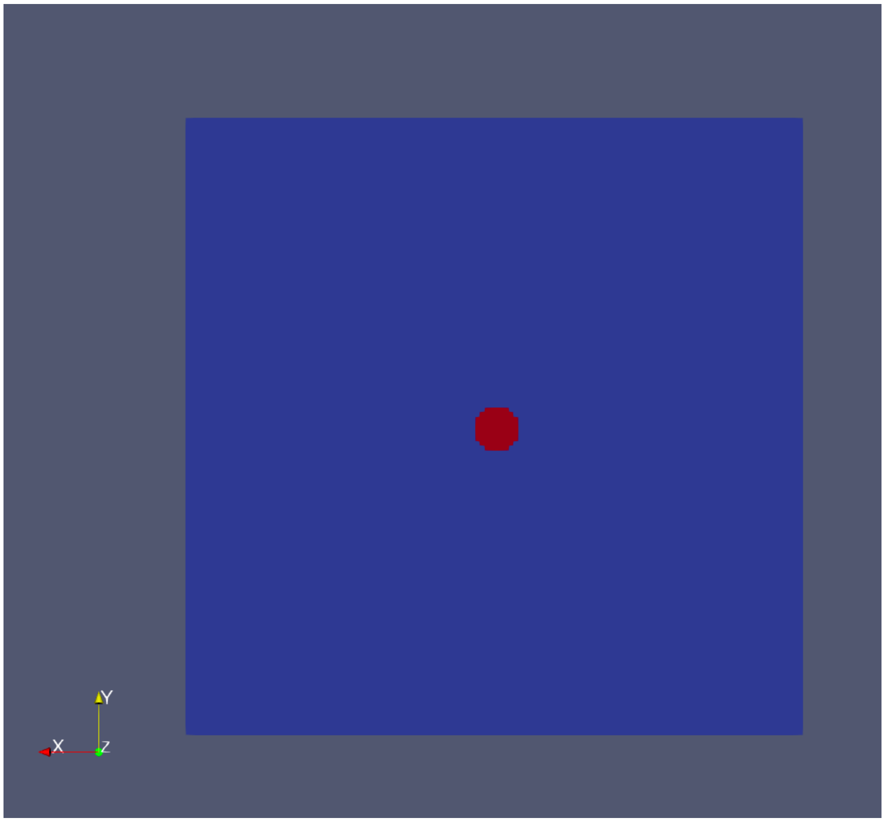
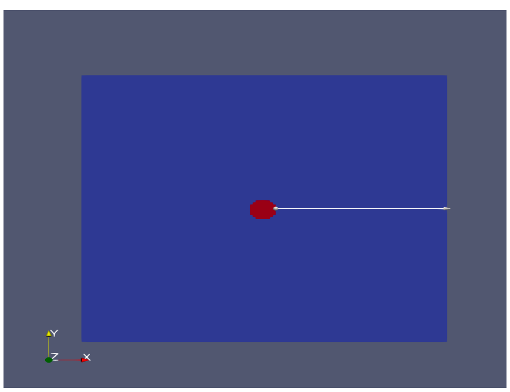
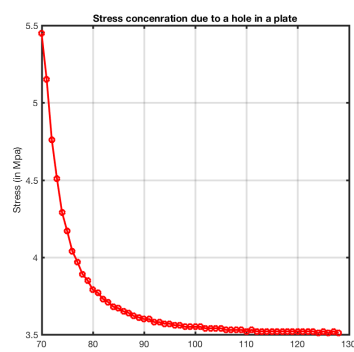


Figure 5: Phase id of microstructure

The σ_{22} stress is plotted along the line as shown in fig. 6.



(a) The line over which σ_{22} is plotted



(b) Stress profile

Figure 6: Stress concentration due to a hole

4 Results

4.1 Different Zener Ratios

We find that the equivalent stress experienced by the material is uniform through out the material for an isotropic material and as the zener ratio increases the percentage of material experiencing an equivalent stress more than the average increases.

4.2 Hole in a plate

The stress at the edge of the hole is more than the nominal stress. This behaviour is as expected. However, the ratio between the stress at the edge of the hole and the nominal is calculated to be 1.57, but theoretically the ratio must be equal to 3. This discrepancy in the calculated value and the theoretical value may be because of the insufficient number of grid points at the edge of the hole and the numerical errors associated with it.