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% Octave program to calculate modulus E
% within [110] plane for MgO
1;

% Function calculates E[hkl] in direction theta
function val = ehkl (theta)
    xp = [-1, 1, 0]/sqrt(2);          % choose x axis in [110] plane
    yp = [0, 0, 1];                  % y axis follows
    vhat = cos(theta) * xp + sin(theta) * yp; % direction vector
    e100 = 247;                       % E[100] modulus value in GPa
    e111 = 343;                       % E[111] modulus value in GPa
    a = vhat (1);                     % direction cosines
    b = vhat (2);
    c = vhat (3);

    % calculate 1/E[hkl]
    tmp = (1/e100) - 3 * (1/e100 - 1/e111) * (a^2*b^2 + a^2*c^2 + b^2*c^2);
    val = 1/tmp;                       % return E[hkl]
endfunction

% create vector of thetas
theta = linspace (0, 2*pi, 200);
nc = columns (theta);
evals = zeros (1, nc);
i = 1;                                % loop to calculate values
while (i<=nc)
    evals (i) = ehkl (theta (i));
    i++;
endwhile

% output the data to a file for plotting
col1 = theta';
col2 = evals';
myfile = fopen("e110.dat","w");
datalength = rows (col1);
i = 1;
while (i<=datalength)
    fprintf (myfile, "%f\t%f\n", col1(i), col2(i));
    i++;
endwhile
fclose (myfile);

```