BANGLADESH UNIVERSITY OF ENGINEERING AND TECHNOLOGY

DEPARTMENT OF ELECTRICAL AND ELECTRONIC ENGINEERING

Course No: EEE 307

Course Title: Electrical Properties of Materials

Assignment: Produce Reduced and Extended Zone Plot of Band Equation

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Section B

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Problem: Produce Reduced and Extended Zone Plot of Band Equation

Solution:

Band Equation: Band Equation is given by the following the equation:

$$\cos(ka) = \cos(\beta a) + \frac{m_o V_0 ba}{\hbar^2} \frac{\sin(\beta a)}{\beta a}$$

Where

$$\beta = \frac{\sqrt{2m_0 E}}{\hbar}$$

For a computer search we construct the equation as,

$$f(E, C) = \cos(\beta a) + \frac{m_o V_0 ba}{\hbar^2} \frac{\sin(\beta a)}{\beta a} - C$$

Where β is a function of E and $C = \cos(ka)$

For each E we search for a k that will give the function f a value close to 0. Then we plot this value for appropriate k in the extended zone.

For reduced zone we apply the transformation,

$$k' = k - n\,\frac{2\pi}{a}, for\ k > 0$$

$$k' = k + n\,\frac{2\pi}{a}, for\ k < 0$$

Where n is given by the equation,

$$n = floor(\frac{ceiling\left(\frac{ka}{\pi}\right)}{2})$$

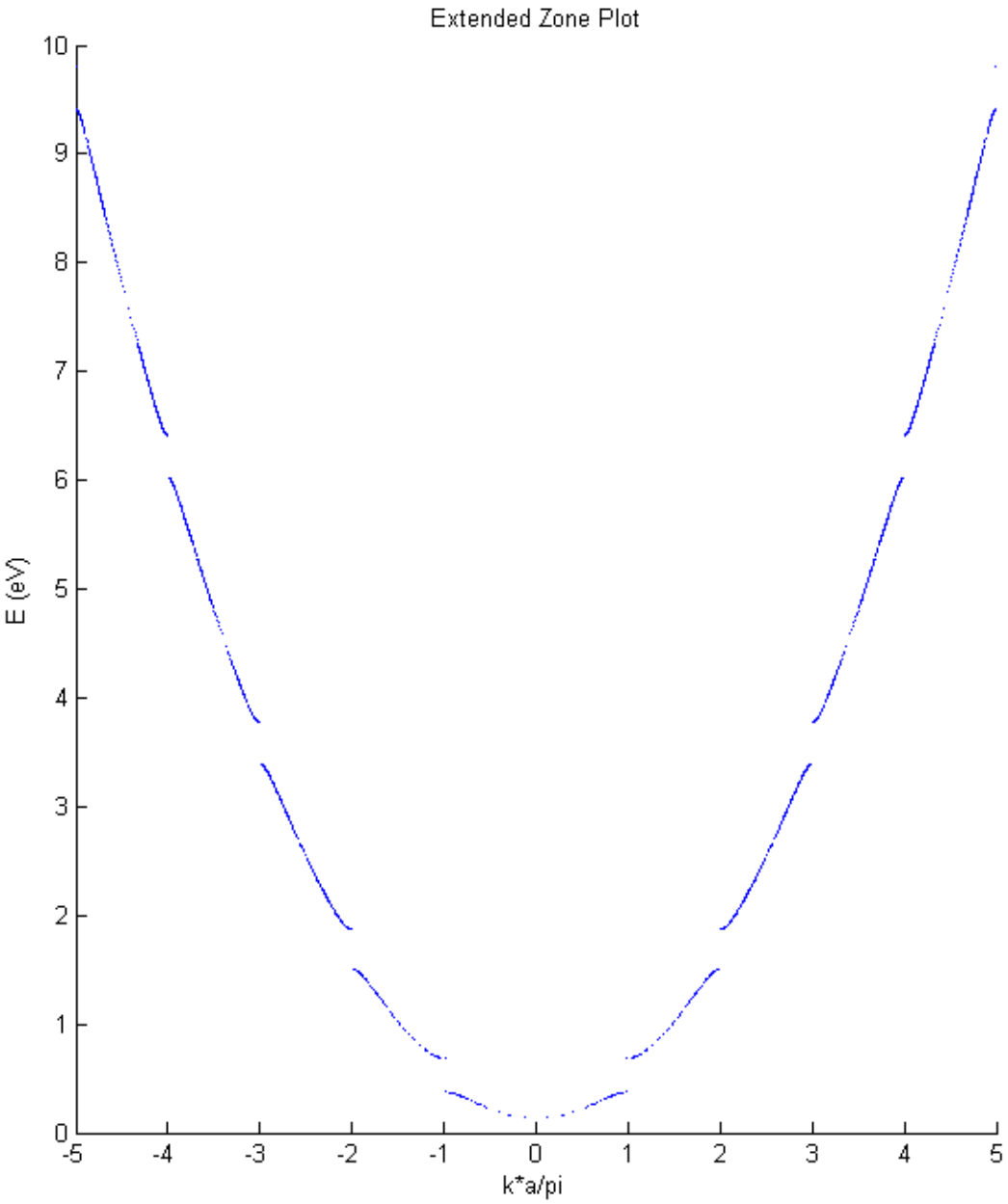
floor is a function that outputs the nearest integer to the left of the point passed in the axis and ceiling is the function that outputs nearest integer to the right of the point in the axis.

Results:

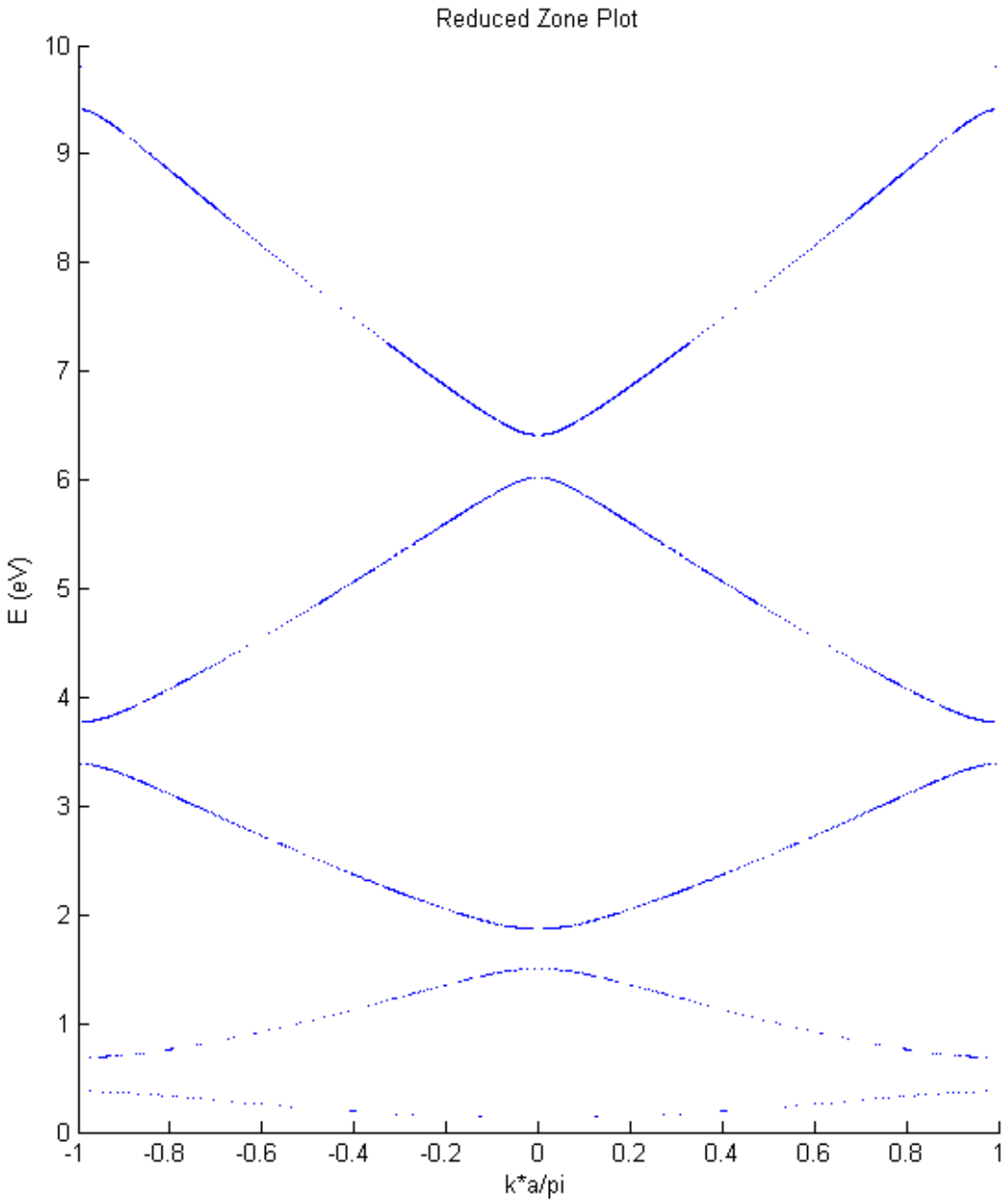
The Matlab plot for the following values is given below:

```
a=10^-9;
b=0.2*10^-9;
V0 = 1.6*10^-19;
```

Extended Zone Plot



Reduced Zone Plot



Matlab Code:

```
%Tariqul Islam, 1006071

clear;
clc;

increment = 10^6; %increment in value of k
steps=5; %upto this value of k*a/pi there will be extended zone plot

a=10^-9; %value of a
b=0.2*10^-9; %value of b
e=1.6*10^-19; %value of electron charge
V0 = e; %value of v0
me=9.11*10^-31; %value of electron mass
hcut=1.05457173 * 10^-34; %value of reduced Planck's constant

P=me*V0*b*a/(hcut*hcut); %value of p
beta=@(E) (sqrt(2*me*E*e)/hcut); %value of beta as a function

f=@(E, coskav) (P*sin(beta(E)*a)/(beta(E)*a)+cos(beta(E)*a)-coskav); %actual
function


%subplot 1 has extended zone plot
subplot(1,2,1);
title('Extended Zone Plot');
ylabel('E (eV)');
xlabel('k*a/pi');
hold on;


%subplot 2 has reduced zone plot
subplot(1,2,2);
title('Reduced Zone Plot');
ylabel('E (eV)');
xlabel('k*a/pi');
hold on;

%extended Zone Plot
E1 = 0; %energy
m=1;
oldk = NaN; %saving the value of k of previous iteration
for m=1:steps
    k=(m-1)*pi/a:increment:(m*pi/a); %values of k
    coska=cos(k*a); %cos ka
    N=length(k); %length of k
    flag = 1;
    %matching each value of E,k to obtain f=0 (under certain tolerance
    %level)
    while 1
        for i=1:N
            if (abs(f(E1,coska(i)))<10^-04) %checking the function
```

```
                if ~isnan(oldk)
                    if (abs(k(i)) < abs(oldk)) %means k has to be increases
%beyond the current limit
                        flag = 0;
                        break;
                    else
                        oldk=k(i);

                        %putting the value in extended zone
                        subplot(1,2,1);
                        plot(k(i)*a/pi,E1,'b');
                        plot(-k(i)*a/pi,E1,'b');

                        hold on;

                        %putting the value in reduced zone
                        min = floor(m/2)*2*pi/a;
                        subplot(1,2,2);
                        plot((k(i)-min)*a/pi,E1,'b');
                        plot((-k(i)+min)*a/pi,E1,'b');

                        hold on;
                        drawnow;
                    end
                else
                    oldk=k(i);
                    subplot(1,2,1);
                    plot(k(i)*a/pi,E1,'b');
                    plot(-k(i)*a/pi,E1,'b');

                    hold on;

                    min = floor(m/2)*2*pi/a;
                    subplot(1,2,2);
                    plot((k(i)-min)*a/pi,E1,'b');
                    plot((-k(i)+min)*a/pi,E1,'b');

                    hold on;
                    drawnow;
                end
                E1=E1+0.0000001;
                break;
            end
            E1=E1+0.000001;
        end
        if ~flag
            break;
        end
    end
end
```

Conclusion:

The values can be varied to obtain different types of plots