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Topic: Density of States in Nanoscale

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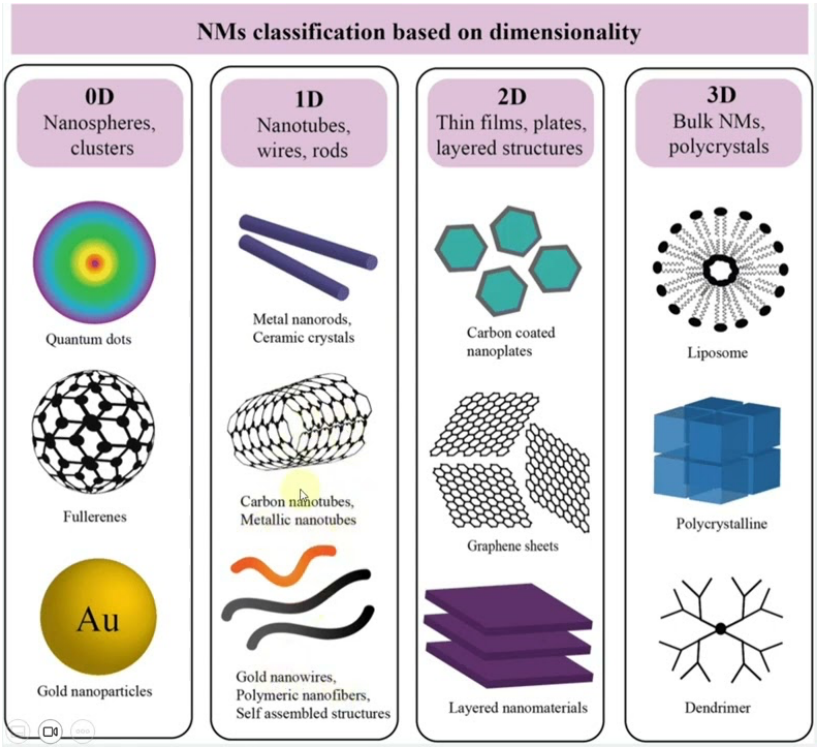
Nanomaterials are the most important element of modern day innovations. A piece of material element which has at least one of its dimensions typically in the range 0 - 100 nm are classified as nano materials. Although the term ‘nano’ originates from a greek word which mean dwarf, the scientific meaning of it is one billionth, i.e. 1/100000000 metres. To have a feeling about its smallness, one can compare it to the dimension of a human hair which is 50000 nanometre on average. The physical property of any material is decided by its constituent elements and the distribution of electrons across various energy states. The number of states per unit energy range is known as the density of states. If ‘dn’ be the number of energy levels per unit volume/area within a energy range of ‘dE’ then the density of states (DOS) is mathematically expressed as $D(E) = dn/dE$. For nanomaterials, DOS strongly depends on the dimension of the material. In nano materials, the nano dimension modify the DOS and this will be discussed in detail below.

The nano materials can be classified into four different category based on the number of dimensions that are in nano regime. These four categories are — (a) 3D, (b) 2D, (c) 1D, and (d) 0D. Here ‘D’ refers to dimension. In 2D nanomaterials, electron can move freely in two dimensions whereas its movement is restricted in one dimension. Similarly in 3D and 1D the electrons can move freely in all three and only one directions, respectively. In most exciting case for 0D, the electrons are confined within nano dimension along all the directions. Examples of all types of nano materials are shown in the figure below. Depending on the type of nano materials ,the DOS also get modified.



Here we will describe the DOS for each type of nano material.

2D DOS: To calculate DOS in two dimension, we need to consider an electron which is confined in two dimensional quantum well. By solving Schrödinger equation for a two dimensional quantum system one can easily find out that each energy state is is dependent on two quantum wave numbers Kx and Ky. As shown in the figure the k-space is a two-dimensional space where each point refers to energy state. The area occupied by each energy state in the k-space is,

$$V_s = (\pi/a)(\pi/b) = (\pi^2/L^2).$$

The circular area in k-space is

$$V = \pi(k^2)$$

As we are only considering the positive values of Kx and Ky, hence only one quadrant area of the circle has to be considered, i.e.

$$V_e = 1/4(\pi)k^2$$

The total number of energy states within one quadrant area become

$$N = [2(\pi)k^2/4][L^2/\pi^2] = k^2L^2/2\pi$$

The factor 2 appears because each quantum state has two electronic states — one for spin up and another for spin down.

Substituting $k^2 = 2mE/\hbar^2$ in the above equation, we get

$$N = 2mEL^2/2\pi\hbar^2 = mEL^2/\pi\hbar^2.$$

By using chain rule we get i.e.

$$dN/dE = (dN/dk)(dk/dE) = mL^2/\pi\hbar^2$$

Hence the density of states in two dimension is

$$D(E) = (dN/dE)/L^2 = m/\pi\hbar^2.$$

The expression for DOS in 2D is thus found to be independent of the energy. It signify that the distribution of energy level is same across all energy values. A more detailed expression for this DOS can be written as

$$D(E) = m[\sum_i H(E - E_i)]/\pi\hbar^2 ;$$

where $H(E - E_i)$ is Heaviside step function. This function will be equals to 1 if E > Ei while it will be 0 if E < Ei.

1D DOS: In one dimension the k-space will be a line. The energy states will be represented by points at equal intervals on the line. The k-space volume of a single state will be

$$V_s = \pi/a = \pi/L$$

K-space volume of the line is = k. Hence, the total number of energy states are

$$N = k/(\pi/L) = kL/\pi.$$

Substituting $k = \sqrt{2mE/\hbar^2}$ in the above equation we get

$$N = L\sqrt{2mE}/\hbar\pi.$$

Again applying chain rule of differentiation, we obtain

$$dN/dE = (dN/dk)(dk/dE) = 1/2(2mL)/[\hbar\pi\sqrt{2mE}] = mL/[\hbar\pi\sqrt{2mE}]$$

The number of states per unit volume per unit energy range is thus given by

$$D(E) = mL/[L\hbar\pi\sqrt{2mE}] = m/[\hbar\pi\sqrt{2mE}] = \sqrt{m/2E}/\hbar\pi.$$

As can be seen in the above expression that DOS in 2D is $D(E) \propto E^{1/2}$. The expression for density of states can be written as

$$D(E) = m^{1/2}/\hbar\pi\sqrt{2E}$$

DOS in 0D: The nanostructure which restrict the motion of electrons in all three directions are 0D nanostructure. Quantum dot is an example of 0D nanostructure. As there is no free motion of electrons, a finite k-space does not exist in this case. All the available states only exists at discrete energy values. Therefore, DOS for 0D nanostructure is expressed in terms of Dirac delta function as follows:

$$D(E) = \sum_i 2\delta(E - E_i)$$

Here the summation is over all i quantum states.

DOS in 3D: In a similar way to the earlier calculation for 2D and 1D nanostructure one can easily find out the volume occupied by one single energy state to be $V_s = (\pi/L)^3$. The total k-space volume in 3D will be $V = 4\pi(k^3)/3$. As we are only interested in the positive k-space therefore only 1/8th volume i.e. the volume in first octant shall be considered. The effective k-space volume is then $V_e = (1/8) * 4\pi(k^3)/3 = \pi(k^3)/6$. Finally, the total number of states within the first octant will be

$$N = 2 * (V/V_s) = \pi(kL)^3/6\pi^3 = (kL)^3/6\pi^2$$

Applying the chain rule of differentiation, we get

$$D(E) = (1/V)dN/dE = (dN/dk)(dk/dE) = [\sqrt{2}m^{3/2}/\pi^2\hbar^2]E^{1/2}$$

As we can see in 3D the density of states is proportional to the square root of energy.

We can now summarise the density of states for all four types of nanostructures as shown below: