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Effect of size and temperature on vacancy concentration in nanomaterials

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Abstract. The study of defects or vacancies helps to understand the transport mechanism that occurs electrically and thermally in materials. It also deals with the mechanical properties of materials. In the present study, the extension of qualitative size-dependent model proposed by Jiang for cohesive energy of nanomaterials is done and size dependence of vacancy formation energy, vibrational frequency and vacancy concentration in nanomaterials is studied. The variation in vacancy concentration in nanomaterials is studied using the extended Jiang model for different dimensional nanomaterials with size and temperature. The model calculations depict the increase in vacancy concentration in free-standing nanomaterials as size of the nanomaterial is reduced and temperature is increased. The behaviour of concentration variation is found just opposite in embedded nanomaterials. The present predicted results of variation in concentration of vacancies follow the same trend as explained in previous studies. The study validates that defects help in the displacement of atoms. The variation in melting temperature and vibrational frequency of nanomaterials with size-dependent vacancy concentration is also discussed.

Keywords. Vacancy concentration; melting temperature; vibrational frequency; size; shape.

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1. Introduction

The nanomaterials are under intense investigation now-a-days because of their world-wide applications in industrial areas. The fascinating and peculiar properties of nanomaterials in comparison to the respective bulk form have attracted the attention of researchers due to more number of surface atoms in nanomaterial and dominance of quantum effects at nanoscale [1–3]. The enhancement in surface area to volume ratio in nanomaterials results in the modification in physical properties in free surface as well as embedded nanomaterials. In free surface nanomaterials, cohesive energy and melting temperature are found to decrease with size reduction due to increase in the number of dangling bonds at the surface with increase in surface atoms [4–6]. Due to the dependence of other thermodynamic parameters on cohesive energy, these parameters also get affected as size of the material varies. Debye temperature of the material depends on its melting temperature and Debye frequency depends on Debye temperature. So these parameters change with variation in size of the material [7–9]. The process that occurs in nanomaterials during mechanical deformation and on increasing the temperature adversely affects the vacancy formation energy and entropy of the material as size varies [10–13].

Point defects or vacancies are created in the material when there is deficiency of atoms in the crystal. Defects affect the electrical and thermal transport mechanism in a material. Also, electrical and thermal properties of the material are greatly affected due to phonon scattering in nanomaterials [14–20]. The size reduction in nanomaterials is strongly linked with vacancy concentration. The energy of vacancy formation and vacancy entropy are the parameters which govern the effect of temperature on vacancy concentration. As number of surface atoms is different in nanomaterials of different dimensions, it is important to consider nanomaterials of different dimensions. During the past decades, various experimental and theoretical studies are done to study the defects in bulk solids and nanomaterials. However, experimental methods are quite difficult [21–23]. It is therefore better to formulate the theoretical model based on thermodynamics to estimate the energy of vacancy formation

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and vacancy entropy in nanomaterials. In this work, the study of defects in nanomaterials is done by extending the thermodynamic Jiang model [24]. The model considered is extended to study the effect of size and temperature on vacancy concentration of nanomaterials. The variation in vacancy concentration in free-standing nanomaterials as well as embedded nanomaterial in metallic matrix is studied. We also determine the variation in vacancy concentration variation nanomaterials with size and temperature. The variation in melting temperature and vibrational frequency with variation in vacancy concentration in naomaterials is studied. The model theory is explained in §2. The results obtained are discussed in §3. Conclusions are given in §4.

2. Mathematical formulations

According to the Jiang model [23,24], the size dependence of the melting temperature is expressed as follows:

$$\frac{T_{mN}}{T_{mB}} = \exp\left\{\frac{-(\alpha-1)}{(D/D_0-1)}\right\}, \tag{1}$$

where T_{mN} is the melting temperature of the nanomaterials, T_{mB} is the melting temperature of the bulk materials, D_0 is the critical diameter. In eq. (1), $D_0 = 2(3-d) * h$ where d is the degree of freedom. For spherical nanoparticle $d = 0$, for nanowire $d = 1$ and for thin film $d = 2$. h represents the atomic diameter of the free-standing nanoparticle.

For free-standing nanomaterials [24], parameter α in eq. (1) is given by

$$\alpha = \frac{2S_{vB}}{3k_B} + 1, \tag{2}$$

where S_{vB} is the bulk vibrational melting entropy and k_B is the Boltzmann constant.

Using the value of α from eq. (2) in eq. (1), the expression of melting temperature for free-standing nanoparticles is as follows:

$$\frac{T_{mN}}{T_{mB}} = \exp\left\{\frac{-2S_{vB}}{3k_B(D/D_0-1)}\right\}. \tag{3}$$

For embedded nanomaterials, the atoms on the surface are not free-standing and parameter α in eq. (1) is calculated as follows [24]:

$$\alpha = \left[\left\{\frac{h_M^2}{h^2}\right\}\frac{T_{mB}}{T_M(\infty)} + 1\right]/2, \tag{4}$$

where h_M is the atomic diameter of the embedded nanomaterial in the matrix and $T_M(\infty)$ is the melting temperature of the embedded nanomaterial in the matrix.

Melting temperature T_{mB} and cohesive energy E_{CB} of the bulk material are related linearly as follows [25]:

$$T_{mB} = \frac{0.032}{k_B}E_{CB.} \tag{5}$$

In view of eq. (1), the cohesive energy ratio in the nanomaterial to bulk E_{CN}/E_{CB} is expressed as follows:

$$\frac{T_{mN}}{T_{mB}} = \frac{E_{CN}}{E_{CB}} = \exp\left\{\frac{-(\alpha-1)}{(D/D_0-1)}\right\}. \tag{6}$$

Lindemann criterion of melting [26,27] relates Debye temperature θ_D and melting temperature T_m of the material as follows:

$$\theta_D \propto (T_m)^{1/2}. \tag{7}$$

In accordance with eqs (2) and (6), cohesive energy of the free-standing nanomaterials is expressed as follows:

$$\frac{E_{CN}}{E_{CB}} = \exp\left\{\frac{-2S_{vB}}{3k_B(D/D_0-1)}\right\}. \tag{8}$$

Considering eqs (1) and (7), Debye temperatures for the nanomaterial θ_{DN} and its bulk form θ_{DB} are related as follows:

$$\frac{\theta_{DN}}{\theta_{DB}} = \left[\exp\left\{\frac{-(\alpha-1)}{(D/D_0-1)}\right\}\right]^{1/2}. \tag{9}$$

Melting temperature varies directly with the energy of vacancy formation as both the parameters follow Fermi–Dirac statistics [11,28]. So, considering eq. (1), the ratio of vacancy formation energy in the nanomaterial E_{vN} to the vacancy formation energy in the bulk E_{vB} is expressed as

$$\frac{E_{vN}}{E_{vB}} = \exp\left\{\frac{-(\alpha-1)}{(D/D_0-1)}\right\}. \tag{10}$$

Expanding eq. (10) up to the first term and using eq. (2), the ratio of the vacancy formation energy in the free-standing nanomaterial E_{vN} to the vacancy formation energy in the bulk E_{vB} is expressed as

$$\frac{E_{vN}}{E_{vB}} = 1 - \left\{\frac{2\,S_{vB}}{3k_B(D/D_0-1)}\right\}. \tag{11}$$

As Debye frequency is directly linked to Debye temperature [28,29] and considering the same for the vibrational frequency, using eq. (9) the ratio of the vibrational frequency of the nanomaterial ω_{vN} to its bulk form ω_{vB} is expressed as follows:

$$\frac{\theta_{DN}}{\theta_{DB}} = \frac{\omega_{vN}}{\omega_{vB}} = \left[\exp\left\{\frac{-(\alpha-1)}{(D/D_0-1)}\right\}\right]^{1/2}. \tag{12}$$

Using eq. (2) and expanding eq. (12) up to the first term, the ratio of the vibrational frequency of the nanomaterial ω_{vN} to its bulk form ω_{vB} for the free-standing nanostructures is expressed as follows:

$$\frac{\omega_{vN}}{\omega_{vB}} = \left[\exp\left\{\frac{-2\,S_{vB}}{3k_{\mathrm{B}}(D/D_0-1)}\right\}\right]^{1/2} = 1-\left\{\frac{S_{vB}}{3k_{\mathrm{B}}(D/D_0-1)}\right\}. \tag{13}$$

Relation between vacancy entropy S_{vB} and melting temperature T_{mB} of the bulk materials is as follows [23,30]:

$$S_{vB} = \frac{3}{2}k_{\mathrm{B}}\ln\left(\frac{T_{mB}}{c}\right), \tag{14}$$

where c is a constant.

Considering eq. (14), vacancy entropy of the nanomaterial S_{vN} is related to the melting temperature T_{mN} as follows:

$$S_{vN} = \frac{3}{2}k_{\mathrm{B}}\ln\left(\frac{T_{mN}}{c}\right). \tag{15}$$

In view of eqs (14) and (15) and eq. (1), S_{vB} and S_{vN} are related as follows:

$$S_{vN}-S_{vB} = \frac{3}{2}k_{\mathrm{B}}\ln\left(\frac{T_{mN}}{T_{mB}}\right) = \frac{3}{2}k_{\mathrm{B}}\left\{\frac{-(\alpha-1)}{(D/D_0-1)}\right\} \tag{16}$$

or

$$\frac{S_{vN}}{S_{vB}} = 1-\frac{3k_{\mathrm{B}}}{2\,S_{vB}}\left\{\frac{-(\alpha-1)}{(D/D_0-1)}\right\}. \tag{17}$$

Putting the value of α for free-standing nanostructures, eq. (17) can be written as

$$S_{vN} = S_{vB}-\left\{\frac{S_{vB}}{(D/D_0-1)}\right\}. \tag{18}$$

At thermodynamic equilibrium, vacancy concentration in the bulk materials $c_{vB}(T)$ at temperature T K is expressed as follows [29,31]:

$$c_{vB}(T) = \exp\left(\frac{S_{vB}}{k_B}\right)\exp\left(-\frac{E_{vB}}{k_{\mathrm{B}}T}\right). \tag{19}$$

In accordance with eq. (19), vacancy concentration of the nanomaterials $c_{vN}(T)$ is expressed as follows [28]:

$$c_{vN}(T) = \exp\left(\frac{S_{vN}}{k_B}\right)\exp\left(\frac{-E_{vN}}{k_{\mathrm{B}}T}\right). \tag{20}$$

Using eqs (19) and (20), the ratio of vacancy concentration in the nanomaterials to bulk is expressed as follows:

$$\frac{c_{vN}(T)}{c_{vB}(T)} = \exp\left(\frac{S_{vN}-S_{vB}}{k_{\mathrm{B}}}\right)\exp\left(\frac{E_{vB}-E_{vN}}{k_{\mathrm{B}}T}\right). \tag{21}$$

Using eqs (10) and (16) in eq. (21), ratio of vacancy concentration in nano to bulk is obtained as follows:

$$\frac{c_{vN}(T)}{c_{vB}(T)} = \exp\left[\frac{3}{2}\left\{\frac{-(\alpha-1)}{(D/D_0-1)}\right\}\right] * \exp\left[\frac{E_{vB}-E_{vB}*\exp\left\{\frac{-(\alpha-1)}{(D/D_0-1)}\right\}}{k_{\mathrm{B}}T}\right]. \tag{22}$$

For free-standing nanostructures, using eq. (2) in eq. (22), ratio of vacancy concentration in the nanomaterials to bulk is given by

$$\frac{c_{vN}(T)}{c_{vB}(T)} = \exp\left\{\frac{-S_{vB}}{k_{\mathrm{B}}(D/D_0-1)}+\left(\frac{2E_{vB}S_{vB}}{3k_{\mathrm{B}}k_{\mathrm{B}}T(D/D_0-1)}\right)\right\}. \tag{23}$$

Taking logarithm of eq. (23) on both sides, eq. (23) can be expressed as

$$\ln\left(\frac{c_{vN}(T)}{c_{vB}(T)}\right) = \frac{2S_{vB}}{3(D/D_0-1)}\left(\frac{E_{vB}-1.5\,k_{\mathrm{B}}T}{k_{\mathrm{B}}T}\right). \tag{24}$$

Using eq. (3) in eq. (24), melting temperature for the free-standing nanomaterials in terms of vacancy concentration ratio in nano to bulk material can be expressed as follows:

$$\frac{T_{mN}}{T_{mB}} = \left\{1-\left(\frac{k_{\mathrm{B}}T}{E_{vB}-1.5k_{\mathrm{B}}T}\right)\ln\frac{c_{vN}(T)}{c_{vB}(T)}\right\}. \tag{25}$$

Considering eqs (12) and (25), the vibrational frequency for the free-standing nanomaterials in terms of vacancy concentration of nano to bulk material can be expressed as follows:

$$\frac{\omega_{vN}^2}{\omega_{vB}^2} = \left\{1-\left(\frac{k_{\mathrm{B}}T}{E_{vB}-1.5k_{\mathrm{B}}T}\right)\ln\frac{c_{v,D}(T)}{c_{v,\infty}(T)}\right\}. \tag{26}$$

3. Results and discussion

In the present study, the dependence of vacancy concentration on the thermodynamic properties of the nanomaterials is discussed. The qualitative expression of cohesive energy of nanomaterials proposed by Jiang *et al* [23,24] is extended in the present study. The expressions of vacancy formation energy, vacancy entropy, vacancy concentration and vibrational entropy for the

Table 1. Input parameters [33,34,36].

Nanoparticles	E_{vB} (eV)	S_{vB}/k_B	h (nm)	T_{mB} (K)
Au	0.95	0.7	0.288	1337
W	3.1	6.5	0.3186	3693
Mo	2.24	5.7	0.3099	2893
Ag	1.13	1.5	0.289	1235
Pb	0.38	1.6	0.350	601

nanomaterials are deduced using Jiang model. The free-standing nanomaterials of Au, W, Ag, Mo, Pb and embedded nanomaterial of Pb in metallic matrix of Al are considered in the present study. The input parameters needed for calculations in free-standing nanomaterials are listed in table 1. The input values required in Pb/Al embedded nanomaterial are taken from refs [38,39].

The vacancy formation energy is observed to vary with size and dimension of the nanomaterial and eq. (11) is applied to study the variation in the vacancy formation energy in Au free-standing nanoparticle with diameter or thickness. The variations in vacancy formation energy of spherical nanoparticle, nanowire and nanofilm of Au are shown in figure 1a using eq. (11). It is observed that vacancy formation energy in free-standing nanoparticles decreases with decrease in size of the nanomaterial. The decrease in vacancy formation energy of Au is maximum in spherical nanoparticles and is least in nanofilms with size reduction. Previous studies reveal that melting temperature in nanomaterials varies linearly with vacancy formation energy of the free surface nanomaterial [20,28,41]. The results obtained from the present calculations for vacancy formation energy of the nanomaterial with size are observed to have the same trend as that of the melting temperature [20,28,32,41].

The relative change in vacancy formation energy of the free-standing spherical nanoparticles of Au, Ag, W, Mo and Pb with reciprocal of diameter or thickness of the nanoparticle is depicted in figure 1b. It is obvious from previous studies [28,41,42] that melting temperature drops on lowering the size of the particle to nanoscale. Due to linear relation between melting temperature and vacancy formation energy, drop in vacancy formation energy is predicted from the present calculations with decrease in size. This decrease is ascribed to the fact that there is increase in surface to volume ratio in free-standing nanomaterials due to increase in dangling bonds at the surface. The variation in vacancy formation energy of free-standing nanoparticle of Pb and embedded Pb nanomaterial in metallic matrix of Al for 1D, 2D and 3D with reciprocal of size is depicted in figure 1c. The tendency of variation in vacancy formation energy of embedded nanomaterial in metallic

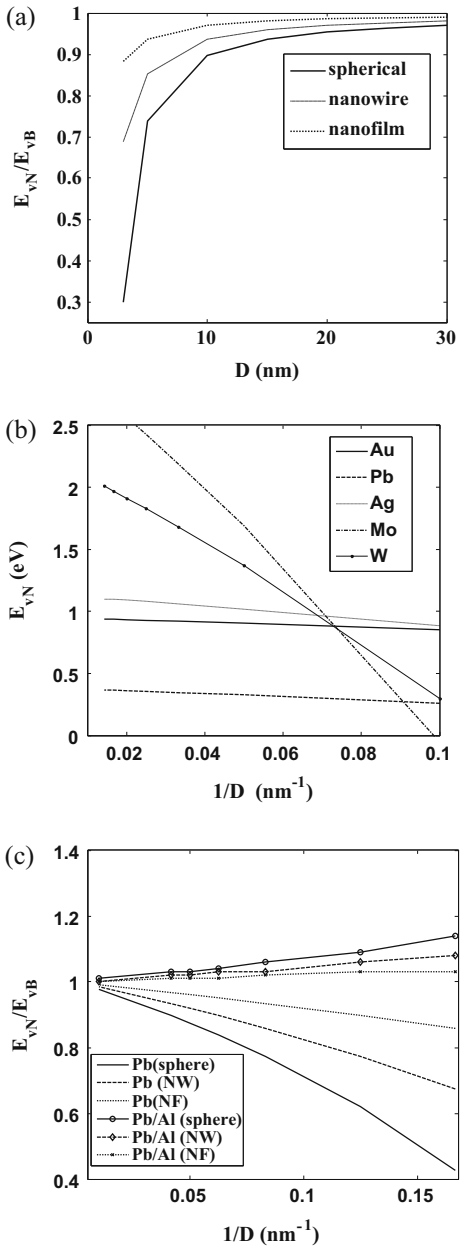

Figure 1. **(a)** Relative change in vacancy formation energy of Au nanoparticles with size, **(b)** vacancy formation energy of Au, Pb, Ag, W, Mo spherical nanoparticles with the reciprocal of diameter and **(c)** vacancy formation energy variation in Pb and Pb/Al nanoparticles with the inverse of the diameter.

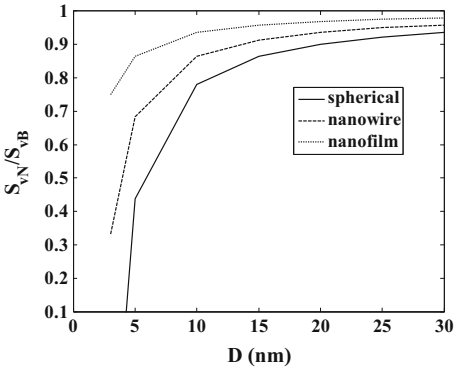

Figure 2. Relative change in vacancy entropy with diameter in Au nanoparticles.

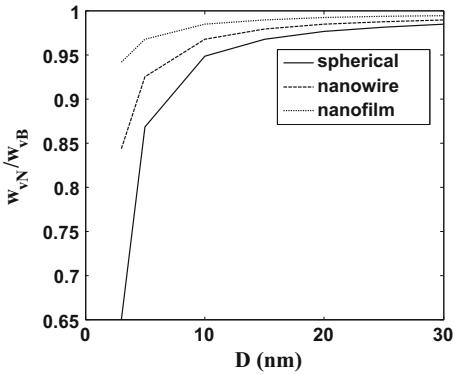

Figure 3. Relative change in vibrational frequency with diameter in Au nanoparticles.

matrix is just opposite to that observed in free-standing nanoparticle. The present results follow the same trend as explained in the available experimental and simulated results for Pb/Al [4–45].

The vacancy entropy variation in nanoparticles with size is studied using eq. (17) in free-standing nanoparticles. Figure 2 depicts the relative variation in vacancy entropy of Au with diameter or thickness for spherical nanoparticles, nanowires and nanofilms. The present predicted results show the relative decrease in entropy with decrease in size of the nanomaterial. It is noted that the present results are in consistency with the results obtained from previous theoretical results [2,14,28,32]. It is clear from the present results that the relative decrease in entropy with size is maximum for nanofilms and minimum for free-standing spherical nanoparticles. The present study shows that vacancy formation energy and vacancy entropy decrease as the grain size is reduced in the nanomaterials.

The increase in the number of surface atoms in nanomaterials results in a drastic change in optical properties of the nanomaterials. There exists a linear relation between Debye frequency and Debye temperature and also between Einstein frequency and Einstein temperature [8,29] and same is true for vibrational frequency. The variation in vibrational frequency with diameter or thickness of the nanomaterial is studied using eq. (13) for free-standing nanoparticles of Au and the results obtained are depicted in figure 3. As melting temperature in free-standing nanomaterials decreases with decrease in size, vibrational frequency is also observed to decrease with size reduction in nanomaterials and the trend followed is the same as in previous studies [46].

The vacancy formation takes place in solids due to the breaking of chemical bonds. As size of the nanomaterial reduces, there is an increase in the number of broken bonds due to the increase in surface atoms, resulting in an increase in vacancy concentration for small size nanoparticles. The vacancy concentration depends on size, temperature, vacancy entropy as well as vacancy formation energy in nanomaterials. The influence of the size of the nanoparticle on vacancy concentration in metallic nanoparticles is investigated at room temperature using eq. (22). It is clear from this study that the vacancy entropy reduces with decrease in size of the nanomaterial and so more vacancies are formed in the material on reducing nanoparticle size to nanoscale resulting in increased vacancy concentration at nanoscale [28,29,35]. Figure 4a depicts the predicted results of relative change in vacancy concentration with diameter or thickness in Au spherical nanoparticles, nanowires and nanofilms at room temperature. It is noted from the results that vacancy concentration increases with decrease in size of the nanomaterial at room temperature and increase in vacancy concentration is maximum in spherical nanoparticles and minimum in nanofilms. Increase in vacancy concentration at nanolevel is supported by the fact that increase in diffusion is found at the nanoscale which helps to increase the vacancy concentration with decrease in size of the nanomaterial as vacancies or defects facilitate the displacement of atoms [30,31,40]. The present results are consistent with the results obtained by other theoretical models [28,32].

Vacancy creation enhances the electrical resistivity of the material and promotes electron scattering [30]. This decreases the efficiency of thermal transport and electron transport and so thermal conductivity in nanomaterials is decreased with the decrease in size of the nanomaterial and therefore the vacancy concentration in the nanomaterial increases on size reduction. By analysing the contribution of vacancy entropy and vacancy formation energy on concentration for different size and temperature as presented in eq. (21), the concentration dependence on size and temperature can be studied. It is noted from eqs (10), (17) and (20) that

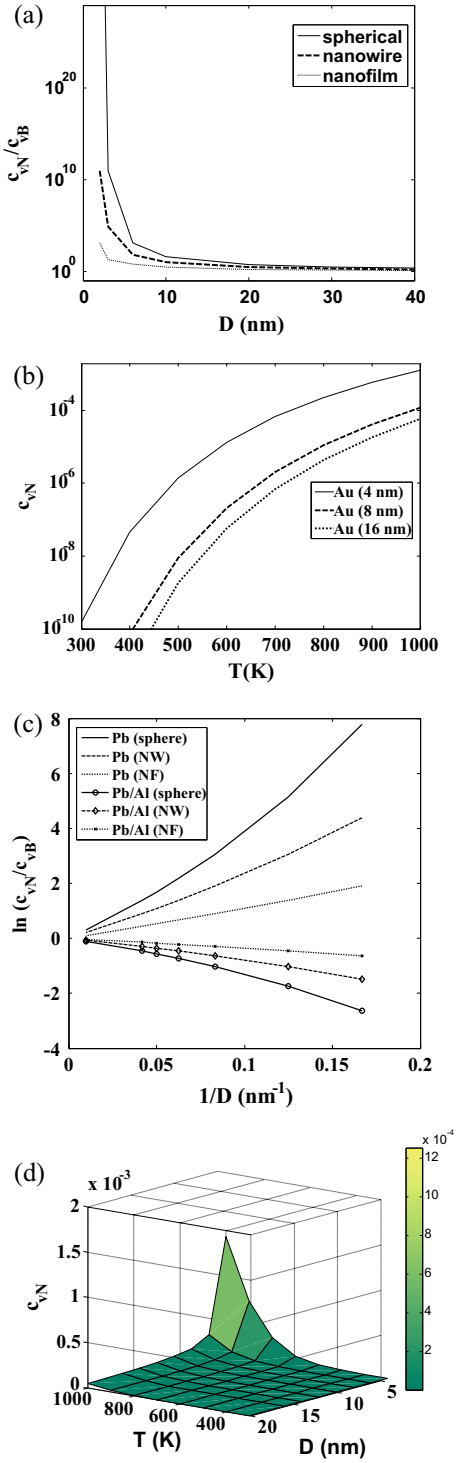

Figure 4. **(a)** Relative change in vacancy concentration with diameter or thickness in Au nanoparticles, **(b)** variation in vacancy concentration with temperature in Au nanoparticles, **(c)** variation in vacancy concentration in Pb free-standing and embedded nanomaterial of Pb in Al matrix with size inverse and **(d)** vacancy concentration vs. size and temperature in Au nanoparticles.

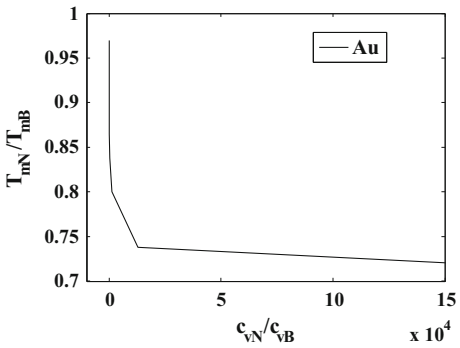

Figure 5. Size-dependent T_{mN}/T_{mB} of Au nanoparticle vs. c_{vN}/c_{vB}.

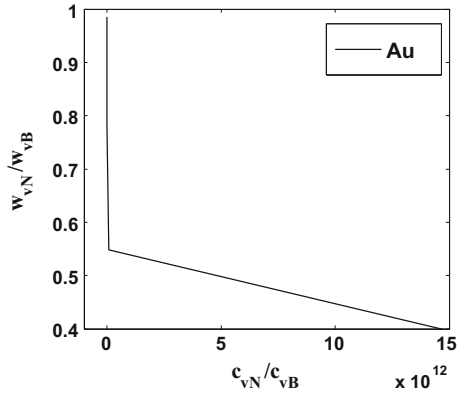

Figure 6. Size-dependent w_{mN}/w_{mB} of Au nanoparticle vs. c_{vN}/c_{vB}.

vacancy formation energy and entropy vary with size in nanomaterials and vacancy concentration depends on temperature. The variation in vacancy concentration of nanomaterials is determined with size and temperature using eq. (20). Figure 4b represents the variation in vacancy concentration in Au spherical nanoparticles of 4 nm, 8 nm and 16 nm diameter with increase in temperature ranging from 293 to 1000 K. It is noted from figure 4b that vacancy concentration in nanomaterials increases with increase in temperature. The present obtained results are consistent with the results obtained by Guisbiers [28] to explain the point defects in nanomaterials.

Variation in vacancy concentration has also been determined for spherical and non-spherical free surface nanoparticle of Pb at room temperature along with embedded nanomaterial of Pb in Al matrix. Figure 4c shows that the tendency of variation of concentration of vacancies with size in free surface nanoparticles is opposite to that in embedded nanomaterial in metallic matrix. In the embedded nanoparticle of Pb/Al, concentration

of vacancies decreases with decrease in size. However, in free-standing nanoparticles, vacancy concentration increases with decrease in size of the nanoparticle. The predicted results follow the same trend as presented in previous studies [32]. To depict the combined effect of size and temperature on concentration of vacancies, figure 4d is plotted in which variation in concentration with diameter and temperature in Au spherical nanoparticle is shown. The results obtained reveal that with increase in temperature and reduction in size, vacancy concentration in nanoparticles increases in nanomaterials. The trend of variation of concentration of vacancies with size and temperature is the same as depicted in previous studies [28].

Figure 5 represents the variation of size-dependent melting temperature ratio T_{mN}/T_{mB} with variation in vacancy concentration ratio c_{vN}/c_{vB} in Au spherical nanoparticles. The reduction in melting temperature has been predicted with reduction in size and increase in vacancy concentration ratio in nanomaterials. Figure 6 represents the variation in size-dependent vibrational frequency ratio ω_{vN}/ω_{vB} with variation in vacancy concentration ratio c_{vN}/c_{vB}in Au spherical nanoparticles. The reduction in ω_{vN}/ω_{vB} has been predicted with reduction in size and increase in c_{vN}/c_{vB} in nanomaterials as vibrational frequency is proportional to the square root of melting temperature and also vacancies created results in reduction in force constants on neighbouring atoms at vacant site and decrease in number of bonding states and so atoms near a vacancy vibrate at lower frequencies [40].

4. Conclusion

In this paper, the influence of size and dimension on vacancy formation energy, vacancy entropy and vibrational frequency of nanomaterials is studied using a quantum approach. The effect of size, dimension and temperature on vacancy concentration is studied. It is found that vacancy concentration in free-standing nanomaterials increases with size reduction and increase in temperature. In embedded nanomaterials, variation in vacancy concentration is just opposite to that observed in free-standing nanomaterials. The effect of vacancy concentration on melting temperature and vibrational frequency of nanomaterial is studied.

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