

Influence of Surface Bonding on Thermo Physical Properties in Silicon Carbide

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Abstract— In this paper we have studied the influence of size and number of atom-pairs in normalized per atom pair binding (cohesive) energy and melting temperature of the Silica carbide (*SiC*) nano-particle using simple model approach. It is observed that the per-atom-pair binding (cohesive) energy and melting temperature are a quadratic function of the inverse of the particle size for *SiC* nano-particle. The per atom-pair binding (cohesive) energy and melting temperature comes near that of their bulk value with increasing the particle size and same as the bulk material when the particle size is above than 100 nm.

Index Terms— Semiconductors; Size effect; Binding energy; Nano-particle; Nano-cluster.

1 INTRODUCTION

In the recent decade, Silicon carbide (*SiC*) is interesting material because of its extremely useful properties, i.e., high stiffness, good electronic properties, high hardness and excellent chemical stability. It has high barrier for electron breakdown, high electron mobility, high thermal conductivity and wide band gap, which is suitable for fabricating high-voltage devices, microwave, solar cell, and radar [1-3]. On with its technological and scientific importance, *SiC* has appealed much attending in the surface science community owing to its specific surface properties. *SiC* nano-crystals (NCs) show unusual surface chemistry and possess special properties [4]. Li et al. [5] have shown that surface charges and quantum confinement play a significant role in determining the optical characteristics of colloidal cubic *SiC* nano-crystals. The thermodynamic properties especially cohesive energy is the significant parameters to understand the nature of bonding in nano-particle. The binding energy is the most practical property to understand the stability of nano-particle and with the help of it we determine the several important parameters such as vapor pressure, melting point etc.. For better interpretation of basic physical properties in small-scale semiconductor materials need to a theoretical study of their cohesive (binding) energies as a function of their particle size that finds out their detailed

dopotential method. Karch et al. [7] have calculated the thermal properties of cubic silicon carbide by first-principles

method. Tang et al. [8] have studied the surface, structural, vibrational, mechanical, and thermal properties of *SiC* by molecular dynamics methods. Park et al. [9] have studied the structural and electronic properties of *SiC* through self consistent ab initio pseudo potential calculations. Farrell et al. [10] have studied that the per atom pair binding energy of small nano-particles and compound semiconductor clusters are quadratic dependence of the particle diameter. They conclude that this variation in size dependence involves the covalent nature of the bonding in semiconductors, and even in the inadequate metals. Recently, Diwan et al. [11-12] have studied the variation of normalized per-atom pair cohesive (binding) energy with size and number of atom-pairs in the BN and InN nano-particle by simple model approach. The possibility of investigating the overall behaviour of nano-particle and cluster depending on its size variation has attracted us to work on this paper.

2 COMPUTATIONAL BRIEF

The binding energy per atom pair (U_{nb}) of nano-particle is defined in the terms of binding energy (U_b) for the bulk crystal and the cube root of the total number of atom-pairs (n) [10]. According to our model approach the binding energy per atom pair (U_{nb}) of nano-particle is expressed as,

$$U_{nb} = U_b \left(1 - 1/n^2\right) \quad 1$$

and the volume of the nano-particle is computed by

$$V_{Total} = 4\pi (d/2)^3 / 3 \quad 2$$

Here d is the diameter of nano-particle. Furthermore the vol-

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atomistic bonding. Chang et al. [6] have studied the structural properties of *SiC* at high and low pressures by ab initio pseu-

ume of a single unit cell of nano-particle is

$$V_{unit} = a^3 \quad 3$$

Where a is the lattice constant of the unit cell. Consequently the total number of unit cells in nano-particle is estimated as

$$N_{unitshell} = V_{total} / V_{unit} \quad 4$$

It is noteworthy that in a face centered cubic crystal, the number of atom pair in unit cell is 2, thus the cube root of the total number of atom-pairs in the particle calculated as

$$n = \sqrt[3]{2(V_{total} / V_{unit})} \quad 5$$

Here Worth of notice that the bulk melting point is proportional to their binding energy for most of semiconductor compounds [17]. Therefore having a similar assumption for the corresponding nano-particle, we can write

$$T_{mn} = T_m (1 - 1/n^2) \quad 6$$

or

$$T_{mn} = T_m [1 - (r_0 / r_n)^2] \quad 7$$

Here r_0 is the average radius of an $n = 1$ particle and $r_n = nr_0$, T_m and T_{mn} is the melting point of bulk crystal and nano-particle, respectively. The average distance (r_0) for face centered cubic crystal can be defined as

$$r_0 = (V_{unitcell} / 2Z)^{1/3} \quad 8$$

3 RESULTS AND DISCUSSION

The input parameters such as lattice parameter (a), binding (cohesive) energy per atom pair (U_b) and melting temperature (T_m) of cubic SiC bulk crystal are reported in table 1. It is known that the large proportions of atoms occupy near the surface in small nano-particles and all on the surface in clusters. So, we have to study the surface configuration in detail that leads the constancy of the particles. Even for bulk materials, parameters that ensure this constancy involving normalized cohesive energy, surface reconstruction, iconicity, bulk structure, melting point hybridization and charge balance. It is worth commenting that many of these factors are quite interdependent. These all factors influence the whole binding (cohesive) energy of particles and give the important information about the deflections from inverse size dependence. The normalization of the energy is defined and computed by the ratio of particle to bulk per atom-pair binding energies, which is also called the energy for a single pair of atoms. The computed normalized per atom-pair (MX) binding energies of SiC nano-particle are shown in Fig. 1-2. It is clear from Fig. 1-2 that per atom-pair binding energies diverge from a linear dependence on $1/n$ (or $1/r_n$) and show an about quadratic dependence on $1/n$ (or $1/r_n$) for SiC nano-particle. As formerly observed, this behaviour is different to the linear dependence determined for most metals [10]. The cause for this fluctuation in size and number of atom-pairs dependence regards the covalent nature of the bonding in semiconductor materials as well as low aspect-ratio metals. The point on the

far left and right in Fig. 1-2 are concerned to the bulk material ($n = \infty$) and single atom-pair ($n = 1$).

It is notable that the binding (cohesive) energy of particle discloses the strength of metallic bond. Our result shows that, decrease in the binding (cohesive) energy of nano-particle means decrease in the strength of the corresponding metallic bond. So it will be easier to break the metallic bond, which will lead to decrease in the melting point of nano-particle. The computed melting temperature (T_{mn}) for SiC nano-particle are shown in Fig. 3-4. It is clear from Fig. 3-4 that the melting temperature (T_{mn}) alter from a linear dependence on $1/n$ (or $1/r_n$) and show a close to quadratic dependence on $1/n$ (or $1/r_n$) for SiC nano-particle.

TABLE 1

INPUT PARAMETERS SUCH AS LATTICE PARAMETER (a), MELTING TEMPERATURE (T_m) AND BINDING (COHESIVE) ENERGY PER ATOM PAIR (U_b) FOR SiC BULK CRYSTAL.

a (Å)	T_{bulk} (K)	E_{bulk} (eV)
4.3596 [13]	3103 [14]	8.13 [15]*

*→ Per-atom pair binding energy calculated from Ref [13]

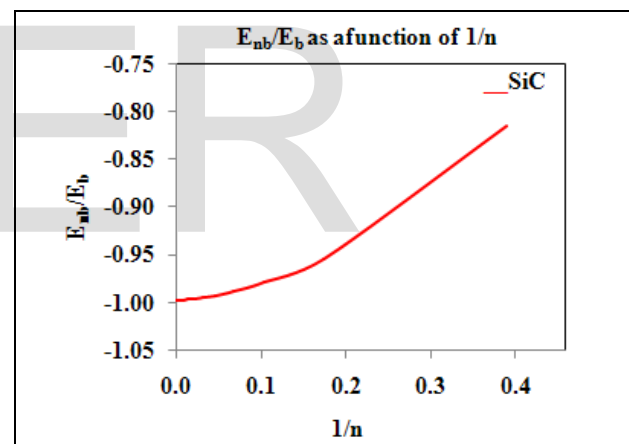


Fig. 1. Variation of relative cohesive energy as a function of $1/n$ for SiC nano-particle.

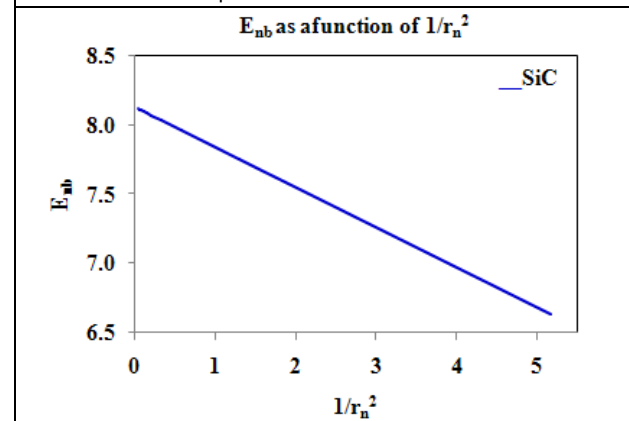


Fig. 2. Variation of cohesive energy as a function of $1/r_n^2$ for SiC nano-particle.

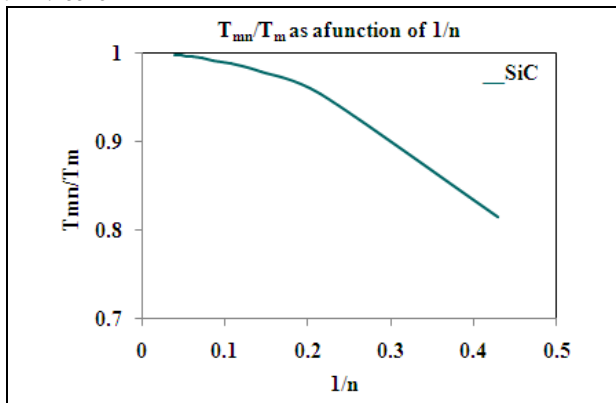


Fig. 3. Variation of melting temperature as a function of $1/n$ for *SiC* nano-particle.

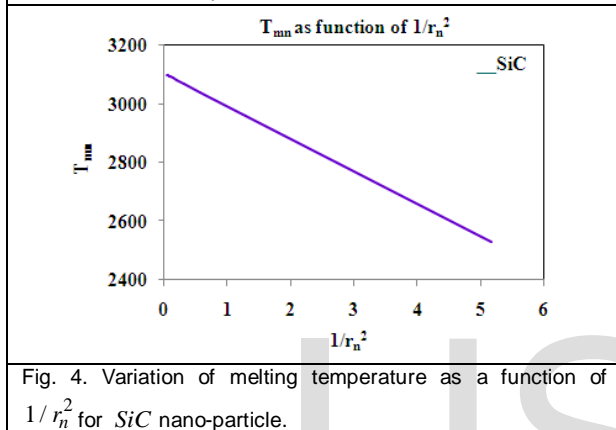


Fig. 4. Variation of melting temperature as a function of $1/r_n^2$ for *SiC* nano-particle.

4 CONCLUSION

An overall assessment shows that the description of the per-atom pair binding (cohesive) energy and melting temperature of Indium nitride (*SiC*) nano-particle attained by us is noteworthy in view of the inherent simplicity of the simple model approach. The model can be considered as the rejoicing approach to explore a variety of factors that influence the cohesive (binding) energies and stability of small-scale and cluster semiconductor. It can be observed that the reports are well fit by a straight line in this size range rationalizing our assumption of a close to $1/n^2$ or $1/r_n^2$ dependence. We hope that the findings of this paper will certainly stimulate the work on the Indium nitride (*InN*) nano-particle and may attract further attention of the experimental scientists in future.

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