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Article

Structures And Bandgaps Of Small Range Gallium Arsenide Nanocluster

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ABSTRACT

There is currently a lot of excitement about Gallium Arsenide nanoclusters due in part to the prediction that small-enough GaxAsy clusters will act as "quantum dot" whose bandgaps can be tuned by varying the cluster size. Small range GaAs clusters (x + y ≤10) were studied by using first principles calculation where structural properties and bandgap were investigated. We obtained the results of bandgap which are larger than the simulated bandgap of bulk GaAs. In this paper, we discuss the effect of GaAs cluster size to the energy bandgap.

| Gallium Arsenide | Nanocluster | Quantum Dot | Band gap |

1. Introduction

Gallium Arsenide nanostructures are being a popular subject of research since last three decades because of its fascinating properties and potential for nanoelectronic devices which is the trend of miniaturization nowadays. Many studies showed that GaAs nanoclusters have a significant change of electronic properties from the bulk. This has been the favor in the fabrication of nano-electronic devices for example, optoelectronic devices and transistors. One of the devices drawing great attention is the Single-Electron Transistor (SET), which has the properties of low-power consumption and high-speed performance. SET consists of a quantum dot with source-drain electrodes as well as a gate electrode. There is currently a lot of effort being made to study the GaAs quantum dots based on the GaAs clusters for their electronic structures.

One of the phenomenons that make nanoclusters or quantum dots become crucial in nanodevices is quantum confinement. It can be observed when the dimensionality of a crystal decreases from bulk to nano dimensions (≤10nm). During this size reduction, the electronic band of the crystal is gradually quantized starting from the band edges as a function of size reduction which consequently results in an increase in the band gap energy (Figure1)[1]. This quantum size effect also results in a blue-shift of energy gap with decreasing size.

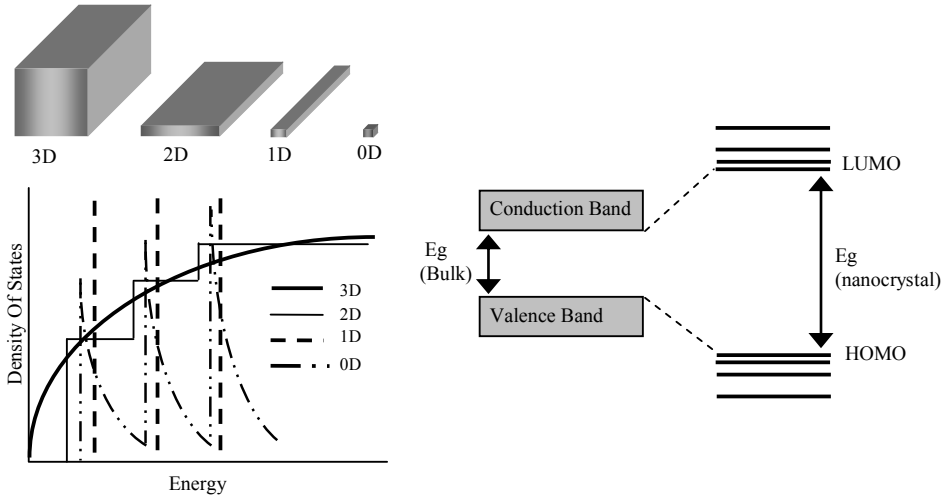


Figure 1: (a) Density of state for different dimension [1]. (b) Difference of electronic states in bulk semiconductor and a nanocrystal [2].

2. Computational Details

The calculations presented here are based on the density-functional theory (DFT) in the local-density approximation (LDA). We employ and implement the code of Vienna ab initio simulation package (VASP)[2-4], which uses plane wave basis set with generalized gradient approximation (GGA)[5] for exchange-correlation functional. The pseudopotentials are combined with the projected-augmented wave (PAW)[6] method which describes the interaction between ions and electrons. A conjugate-gradient (CG) [7] algorithm is used to optimize the atomic structures.

In order to simulate an isolated cluster, supercell approach is implemented. Supercell size of 1.6nm was used to omit the interaction between the clusters and its periodic image in 3D. We use a cutoff energy of 250eV for the plane wave expansion to ensure precise results obtained. Gaussian smearing of 0.1eV was used in order to perform the density of states. Owing to the supercell approach, the cluster calculations are performed using the Γ point only. Before the electronic structures simulations, the structure of the GaAs clusters is allowed to be optimized in the self consistent cycle. After the structure optimization, band structure calculations are performed.

3. Results And Discussion

Figure 2 shows the lowest-energy structures of each Ga_xAs_y ($x + y \leq 10$) which are also the most stable structure. Calculations find the symmetry group of C_{2v} linear for GaAs, C_{2v} triangle for Ga_1As_2, D_{2h} planar rhombus for Ga_2As_2, C_{2v} trigonal bipyramid for Ga_2As_3, C_1 capped trigonal bipyramid for Ga_3As_3, C_s capped prism for Ga_3As_4, C_1 rhombic prism for Ga_4As_4, C_s tricapped trigonal prism for Ga_4As_5 and C_s tetracapped trigonal prism for Ga_5As_5. The structures of Ga_xAs_y ($4 \leq x + y \leq 6$) is built according to edge-capping mode while face-capping growth mode is preferred for Ga_xAs_y ($7 < x + y < 10$) [8].

The accuracy of the calculation is tested first for bulk Gallium Arsenide. For the zinc blende structure GaAs with lattice constant 5.653Å which is close to experimental lattice constant 5.632Å, the band gap obtained from the simulation is 0.5453eV which is lower than the experimental result. This is because density functional is a ground state theory and thus it underestimated the band gap value.

Table 1 shows the energy versus bandgap (highest occupied molecular orbital - lowest unoccupied molecular orbitals gap) of Gallium Arsenide clusters with different number of atom. Overall, the bandgaps of Gallium Arsenide nanocluster Ga_xAs_y are larger than the bulk Gallium Arsenide. It shows that when GaAs reduces to nanosize, its properties will change where the bandgap will increase. According to quantum theory, the bandgap increases as the size decreases. This indicates the stronger confinement for the smaller sizes. However, Figure 3 shows the results that do not comply with the above theory. Instead, it changes unevenly up and down between 0.7370 eV to 3.0956 eV. However, our results are in good agreement with those reported in literatures [10]. Among these nanoclusters ($x + y \leq 10$), GaAs is observed to posses the highest bandgap energy whilst Ga_4As_5 has the lowest value.

We can say that when the size of the cluster is very small (< 1nm), the bandgap energy does not increase with the decreasing of size. However, with the widening of the bandgaps from bulk, small GaAs clusters are still showing their evolvement and difference from bulk as size reduction. The bandgap depends strongly on the number of atoms and atomic structure. For a structure with the same number of atom but different configuration, the bandgap might be different.

So, the results can be used to predict the performance of the SET. When the cluster between the source and drain becomes smaller in size, the energy gap increases which means the confinement effect is stronger. This can optimize the operating temperature of SET because of the relation $E > kT$, where E is the energy similar to the energy spacing of quantum dot. Besides that, we can predict the I-V characteristic of SET by understanding the energy level of the quantum dot and that we can know how much energy should be applied to pass quantized electrons.

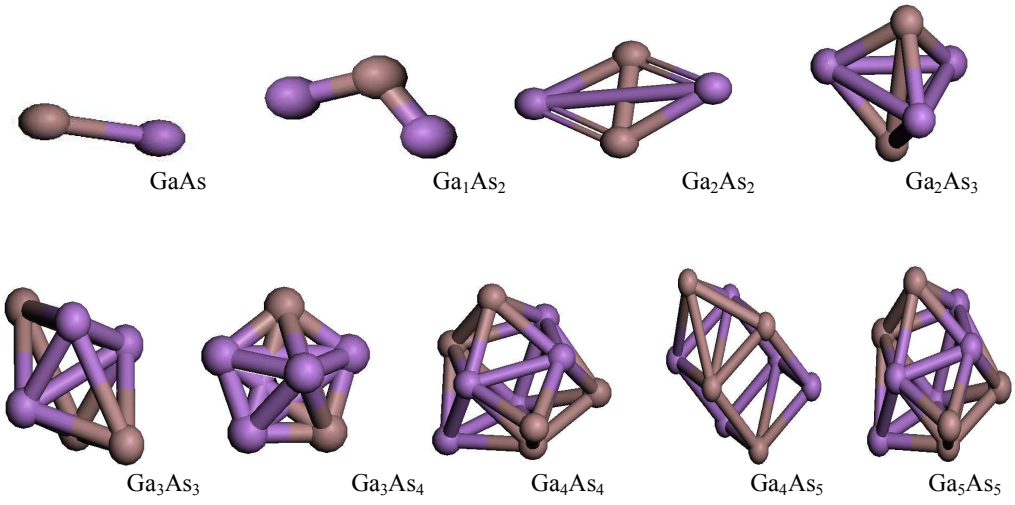


Figure 2: Lowest energy structures of Ga_xAs_y

Ga_xAs_y	Symmetry Group	Bandgap energy (eV)
GaAs	C_{2v}	3.0956
Ga_1As_2	C_{2v}	0.8756
Ga_2As_2	D_{2h}	1.4031
Ga_2As_3	C_{2v}	1.0918
Ga_3As_3	C_1	1.6689
Ga_3As_4	C_s	1.5755
Ga_4As_4	C_i	1.0062
Ga_4As_5	C_s	0.7370
Ga_5As_5	C_s	1.5898

Table 1: Calculated structure and ban GaAs ($x+y \leq 10$)

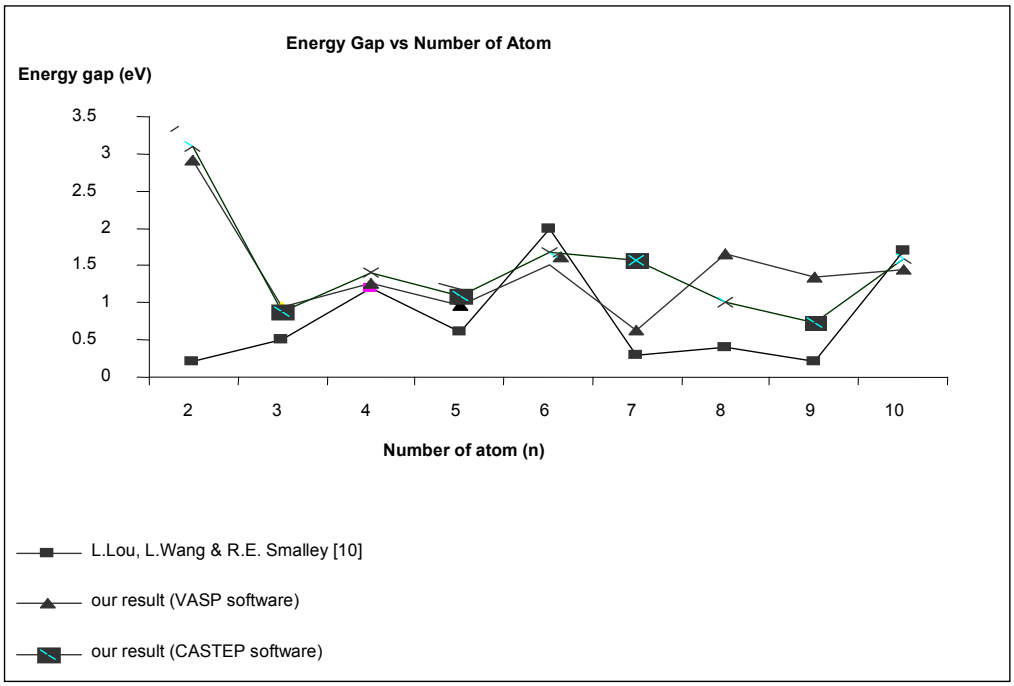


Figure 3: Bandgap (HOMO-LUMO) for Ga_xAs_y gap for each

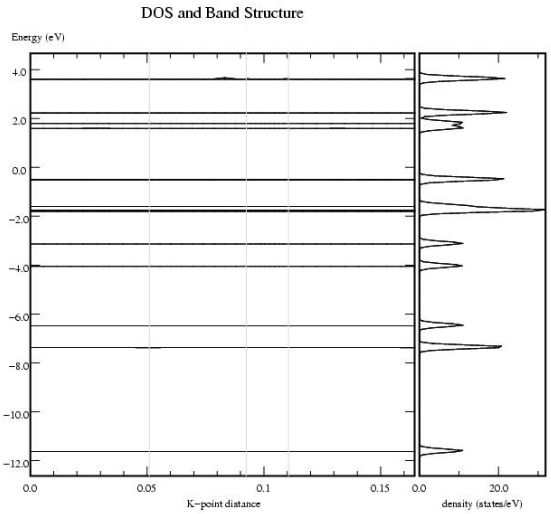
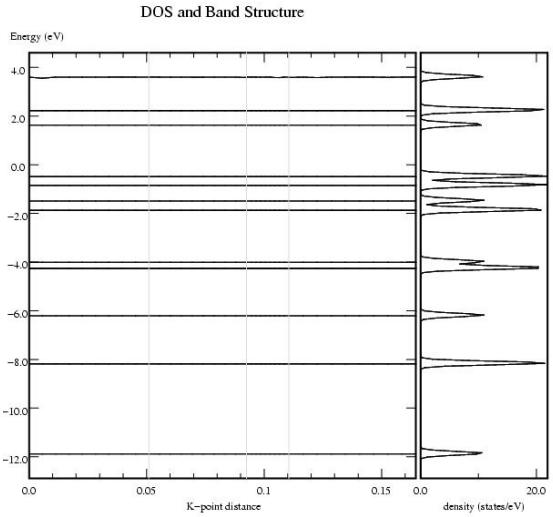


Figure 4: (a)Typical bandstructure of GaAs



(b) Bandstructure of Ga_3As_3

4. Conclusion

Calculation using DFT and LDA shows bandgap energies of gallium arsenide clusters are larger than bulk gallium arsenide. It shows that electronic properties of nanocluster are differing from the bulk where bandgap widening is observed. Bandgap values change between 0.7370 eV to 3.0956 eV. It depends strongly on the number of atoms and atomic structure.

5. Acknowledgement

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