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Surface Structure for Silicon Nanoparticles

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ABSTRACT

A model depend on ratio number atoms of the Surface to the internal atoms used to calculate the mean bonding length ($d_{mean}(r)$) of silicon nanoparticles with radius (r) in the range of ($1.2nm \leq r \leq 10nm$). The results compared with the ($d_{mean}(r)$) which measured from high resolution transmission electron microscope (HRTEM) in the range of (r), using AUTO CAD software for measuring nanoparticle radius and the spacing between adjacent fringes that correspond to d_{hkl} – spacing. The results obtained that the theoretical model is in good agreement with the experiment for all (r) range. The lattice parameter ($d_{mean}(r)$) are found to increases from (0.235nm) for bulk Si up to (0.262nm) for nanoparticles having a size down to 3nm, then it is increased sharply at about the critical radius of silicon nanoparticle (r = 1nm), which related to the atomic surface behavior.

1.Introduction:

Semiconductor nanoparticles have received much interest recently as a useful class of materials for future optical and electronic devices [1]. Is due to properties related to the effects of quantum confinement , which occur when the particle size approach to the excitonic diameter of electron- hole pairs in the semiconductor Material [2].

Nanocrystals are the Fundamental bulding blocks for the nanostructures and devices. In particular for optoelectronic application quantum confinement effects and the role of surface states for crystals smaller than 10 nm are of particular interest[3].

The bulk materials properties are typically constant with change the Size , while nanomaterial give size dependent physical and chemical properties [4]. In general, the size of a nanoparticle spans the range between 1 and 10 nm [5].

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The lattice parameter is very important quantities in a material structure which effect on physical and mechanical properties that the lattice parameter of nanoparticles depends on the particle size [6-9]. For example, the lattice constant of Au nanoparticle decreased by 0.3% with a diameter of 2.5 – 14 nm [10]. The lattice constant of Si increased from 0.237 nm to 0.282 nm with r change from 9.94nm to 1.93 nm [11].

For nanoscale materials, Group IV Semiconductors with nanoscale materials such as Si and Zn , bonding length are increases with particle Size decreasing.To find the lattice parameters of the nanomaterial experimental for each size is nearly difficult, so a simple formula my found to determine the lattice parameters of the nanomaterial. The aim of this project is to measure the mean bond length ($d_{mean}(r)$) for Si nano-particles from high-resolution transmission

electron microscopy (HRTEM) and comparing them night those. Calculated from the equation of nanosize dependence of lattice volume.

2. Methods of calculation:

The average distance between the two bonded atoms is defined as the bond length .the bond energy value depend on the bond length , where the shorter bond length is the larger bond energy. Also the bond length depend on the size of atoms, which increases with it [12]. for nanoscale range the $d_{mean}(r)$ increases with the decrease of radius (r) of the nanoparticle to d_{mean} (r_c) which the maximum Value , where r_c is the critical value which equal to 3h , where h is the height of the first solid surface [13].

For the nanoscale the lattice volume depend on the mean bond length of the surface d_{mean} (r_c) = h , while, for a bulk (r = ∞), the lattice volume depends on $d_{mean}(\infty)$, To calculate the mean bond length $d_{mean}(r)$, using the following relation [11].

$$d_{mean}(r) = h - \Delta d_{mean}(r) \qquad (1)$$

Where

$h = 1.429\, d_{mean}(\infty)$

and $d_{mean}(\infty) = 0.235$ nm for Si [13]

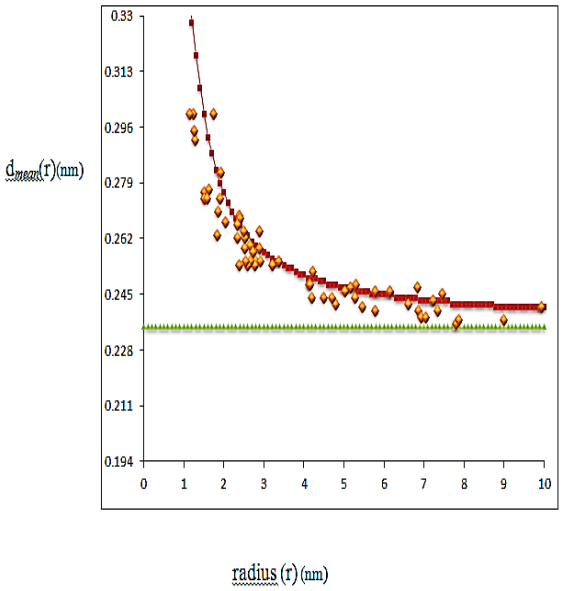
The size-dependent of mean bond length $d_{mean}(r)$ should be result of its dependence on n_s/n_v, where n_s and n_v are the numbers of surfaces and interior atoms, respectively. The best size dependent of $\Delta d_{mean}(r)$ are given in the following relation [14]:

$$\Delta d_{mean}(r) = \Delta d_{mean}(r_c)\left[exp\left(\frac{-2(S_m-R)}{3R\left(\frac{r}{r_c}-1\right)}\right)\right]^{\frac{1}{2}} \qquad (2)$$

Where R is the ideal gas constant and equal to ($8.3149*10^3$ J/K.mol) and $S_m(\infty)$ is the bulk overall melting entropy, equal to ($29.48\ J \cdot K^{-1} \cdot mol^{-1}$) for Si [14]. Thus using equation (2) in equation (1) to became:

$$d_{mean}(r) = h - \Delta d_{mean}(r_c)\left[exp\left(\frac{-2(S_m-R)}{3R\left(\frac{r}{r_c}-1\right)}\right)\right]^{\frac{1}{2}} \qquad (3)$$

So the value of d_{mean} (r) calculation as function of (r) in the range between (1.2– 10nm), using a software program as shown in figure (1).



Figure(1). Variation of lattice parameter versus diameter for silicon nanoparticle. The solid curve in terms of Eq(5) the dashed line denoted bulk lattice parameter($d_{mean}(r)$) of silicon which is equal to 0.235 nm, experimental results shown as ♦,

Figure (1) indicates that the lattice parameter ($d_{mean}(r)$) increases with decrease in the diameter of *Si NP* until reach to critical size (radius) at which all atoms are located on the surface, it is equal to ~1nm for *Si Nps*, respectively.

3. Methods of measurement:

One of the most powerful methods of direct structural analysis and determining the lattice constant of nano solids are provides by *HRTEM*. The diameter of *NPs* is defined as the diameter of the circle equivalent to the area of the *NP's* image. Better accuracy has been obtained when the measurement is averaged over more measurable lattice planes, and source of error here are limited to the ability of locating software's calibration at the center of lattice planes and also visibility offered by the software used. Nanoscaled particles give the fundamental and technological properties , which determined by their structure and size. High-resolution transmission electron microscopy (HRTEM) using the aberration-corrected Titan 380-300 microscope allows detailed studies of cluster morphologies.

In order to obtain fast work and more precisely, AUTO CAD software was used for measuring the diameter and spacing between adjacent firings that correspond to d_{hkl}-spacing.–It is important to the existence of a scale bar on the original images, without it measuring process cannot be obtained. When the image loaded on the software, the magnification also should be the same for both dimensions x- and y-axis, in order to avoid distorted images caused by different magnification in the x- and y- directions. The values of measurable scale bar have been used as a reference to the other measurements, such as d_{hkl}-spacing and nanocrystals sizes. Figure(2). obtain the HRTEM image of Si-nanoparticle prepared by de-magnetron sputtering technique [15].

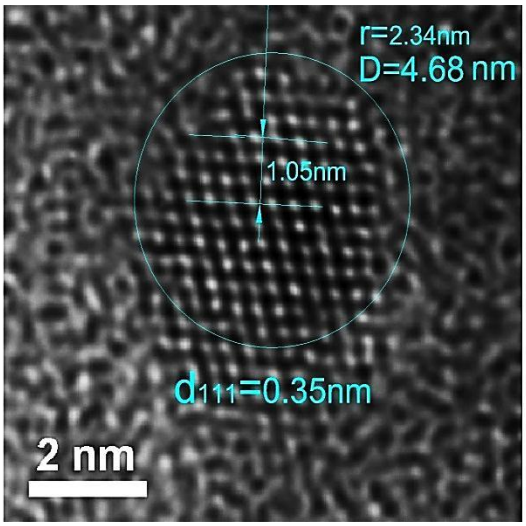


Figure (2) Typical *HRTEM* images, measuring d_{hkl}-spacing and size directly on *HRTEM* image of *Si NP* [15], of diameter ~ 4.68 nm, the period of the fringes observed in the *NP* corresponds to the d_{hkl}-spacing of the (111) plane and it is found to be ~ 0.35nm.

This work d_{hkl}-spacing for the nanoparticles of different sizes are investigated, correlation between their diameter and lattice constant can be made by applying

$$a = d_{hkl}\sqrt{h^2 + k^2 + l^2} \qquad (4)$$

and

$$d_{mean}(r) = (a/4)\sqrt{3} \qquad (5)$$

The value of $d_{mean}(r)$from the experimental results are shown in figure (1).

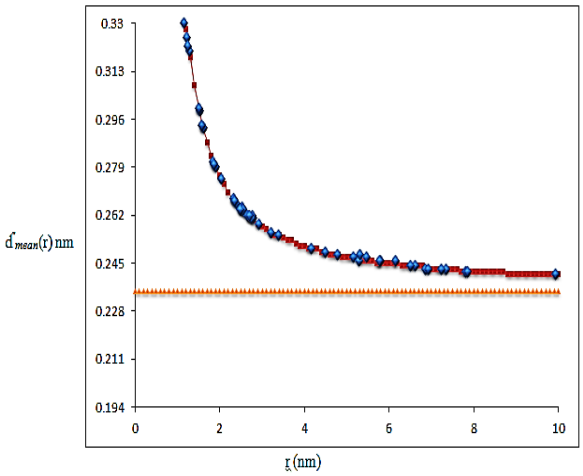
4. Results and analysis:

Measured values of $d_{mean}(r)$ obtained from HRTEM images of surface Si nanoparticles are well agreed with those calculated from equation (3). Shown in figure (1), which obtained that $d_{mean}(r)$ increased with decreasing the Si nanoparticle radius this increasing became sharply at about the critical

radius of silicon nanoparticle (r = 1nm), which related to the atomic surface behavior. The increasing of $d_{mean}(r)$ with decreasing (r) may be related to many factor the first, When the crystal size at the nanoscale range , the surface to bulk ratio will be high and the bonding length of the surface is much larger than bonds of the bulk material [6,8]. The second, can be explain the d_{mean} increase, may be related to the forces on the atoms surface [16],where the surface atom experience nan-zero forces which are induced by the breaking process in the surface formation induces forces which push the outer larger atoms out of their bulk position and the third may be according to the effect of materials metallic [14], Where ,the bond length of Si increasing due to the metallic properties of compound with more polarizability. The experimental point of d_{mean} were not layer on the carve due to Eq.(3) their deviation may be related to the examined crystal angle by HRTEM to give another d_{mean} (r)value, so the correct d_{mean}i.e (d'_{mean} - d_{meam} = 0), The real values of d_{mean} (r)are corrected by using relation

$$\text{Cos } \theta = d'_{mean} / d_{mean} \qquad (7)$$

The correct curve of d'_{mean} with particle radius obtained is as shown in figure (3).



Figure(3). Variation of lattice parameter $d'_{mean}(r)$ versus radius for silicon nanoparticle. The dashed line denoted bulk lattice parameter of silicon which is equal to 0.235 nm, experimental results shown as ♦.

5. Conclusion:

1. The calculated mean bonding length of silicon nanoparticles using a model free from fitting parameter was found to be in good agreement with the experimental data obtained directly on the HRTEM image of Si Nps.

2. Mean bonding length increases with decreases the radius of Si Nps, until reach to critical radius of 1nm.

3. The shift in examined crystal angle by HRTEM for Si Nps increased with r at r ≤ 3nm, by the same behavior of d_{mean}.

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التركيب السطحي لجسيمات السيكون النانوية

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الخلاصة :

صمم برنامج لحساب نسبة عدد ذرات السطح الى عدد الذرات الداخلية لحساب معدل طول الاصرة لجسيمات السياكون النانوية لمدى نصف قطر بين (1.2- 10 nm). ومقارنة النتائج المستحصلة مع نتائج معدل طول الاصرة المحسوب من القيم التجريبية للمسافة البينية المأخوذ مباشرة من فحص المجهر الالكتروني علي التحليل (HRTEM) بإستخدام برنامج حاسوبي نوع (AUTO CAD) لقياس نصف قطر الحبيبة والمسافة بين الاهداب المتعاقبة لتعطي قيمة d_{hkl}.النتائج اظهرت بأن البرنامج النظري يتطابق مع العملي بشكل جيد ولجميع قيم نصف القطر (r). ان قيم معدل طول الاصرة يزداد من(0.235nm) للسيكون السميك تصل الى(0.262nm) ان قيم معدل طول الاصرة يزداد مع نقصان نصف القطر بشكل تدريجي والى قيمة (r = 3nm) حيث الزيادة تكون حادة ولقيمة نصف القطر الحرج للسيليكون النانوي (r=1nm) والتي تعود الى سلوك ذرات السطح