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Research Article

THE EFFECT OF CRYSTALLINE LATTICE OF NANOPARTICLES ON MANUFACTURING

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ABSTRACT
Nanotechnology is a kind of technology to produce materials and tools in nano scale. In recent years, this branch of science is used more to find a solution for energy crisis and environmental pollution. Using new technology especially nanotechnology in order to lessen the negative effect of pollution on environment, proposed as one of the administrative approach. In this paper, at first, all kinds of nanoparticles are introduced. Secondly, some especial characteristics of nanoparticles that help us more to know them are briefly explained. Thirdly, nanoparticles which can use to produce Nano filters are studied and the way of nanoparticles application is presented. Then, crystalline lattice of used nanoparticles in Nano filters is investigated. Because solid nanoparticles have a particular structure, they can use to make improvements in nano filters. So, in this article, we tried to gather all required information and the effect of solid state characteristics on nanoparticles.

***Keywords**: Nano Filter, Nanoparticles, Crystalline Lattice, Face Centered Cubic Structure*

INTRODUCTION
Nanotechnology has an ability to produce new materials, devices and systems because it can control the properties of them that are depended on molecular and atomic surface. Nowadays, the entire world is improving and changing by using nanotechnology science. It seems to be advantageous that gathers necessary information in order to study, investigate and know nanotechnology and its useful and harmful effect on environment. Nanoparticles are being used in all fields around us like, chemistry, physics and clean energy. The combination of Nano science and technology is called nanotechnology. Nanotechnology is useful to solve many problems. In addition, it was used to manufacture or improvement of past inventions. Now, one of the most important problems in this word is Global warming that can be raised from overusing of fossil fuels which caused air pollution. Air pollution and Global warming are the most serious reason to Greenhouse effect. One of these problems is that if we are continuing to consume fossil fuels, soon there will be no more fuels to use. One of the most important usages of nanoparticles is that they can produce better fuels and for this reason they can reduce the consumption of fuels. In addition, Nano filters can prevent entering contamination of consuming fossil fuels into air. These cases are slight application of using nanoparticles and nanotechnology. Using nano filters let us to make possible the separation of solution which is included both advantageous and disadvantageous component. Nano filtration use permeable membranes for separation. Normally, these membranes consist of two layers. Thin and dense layer are applied to separate and protective layer protect whole system from pressure. Membranes have different shapes such as: spiral, plane, tube and fiber. Nano filtration is prevalent during recent years. In Nano filtration, isolation is done based on the size of molecules. Basically, in this procedure, in order to omit organic component such as: contaminations in micro size and polyvalent ions. Other application of this nanostructure is that enable us to mention omitting chemical materials which are used to kill harmful organisms from water, elimination heavy metals such as: Mercury, water treatment, decolonization and omission of contamination. Nano filtration can create clean water from any kind of water source and eliminate all bacteria in water.Studying Nano filters better requires to know structure of them, substances which they made up from and properties of

substances. As regards that the role of crystalline lattice is clear in many sciences; it is suitable to review the effect of crystalline lattice on Nano filters.

Each scientific improvement that happens in the world should be investigated, because some improvements besides their advantageous can be harmful too. Nanotechnology is not an exception. So, whatever we know more about nanoparticles and their useful and harmful effects, we could use them better.

INTRODUCING NANOPARTICLES AND THEIR KINDS

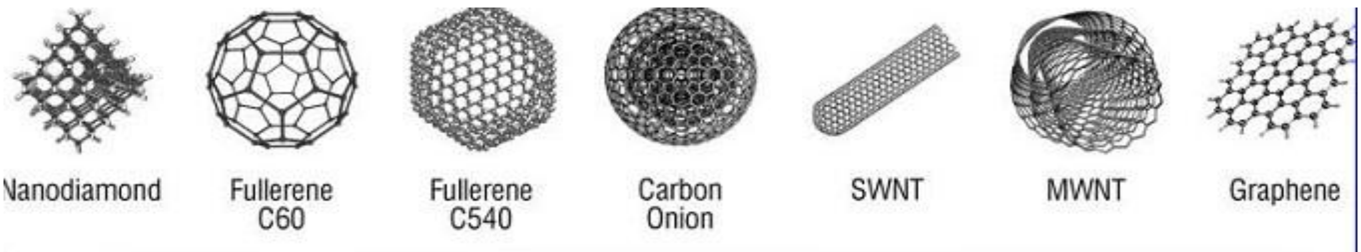

Figure 1: Kind of Nanoparticle

Nano particle is the kind of particle in the scale of 1 to 100 nanometer. Nano particles can be categorized in three main groups (See Fig. 1.): 1) Carbon-based material such as fullerenes and carbon nanotubes, 2) inorganic nanoparticles are based on metal oxides (Zinc oxide, Iron oxide, Titanium dioxide and cerium oxide, etc.) and metals (gold, silver, iron) and 3) quantum dots such as cadmium sulfide and cadmium selenide. Mixture of different phases can also manufacture nanoparticles.
In addition, these nanoparticles have different and interesting morphologies such as spheres, tubes, rods and prisms. Nanotechnology includes the integration of these Nano scale structures into larger material components and system, keeping the control and construction of new and improved materials at the Nano scale (Roco and Brainbridge, 2001), (Rosi and Mirkin, 2005) and (Rotello, 2003). The difference between nanoparticles and their bulk is in the case of the number on surface atoms and also their properties that caused from the surface volume ratio of NPs. some properties of bulk materials such as density, specific resistivity, magnetization ability and dielectric constant for nanoparticles are just an average of bulk one but some of the properties of NPs are completely changed. These changes are due to decreasing the size up to nanometer and increasing the number of surface atoms (Daniel and Astruc, 2004) (Niemeyer, 2001).

CHARACTERISTICS OF NANOPARTICLES

Complete characterization of nanoparticles includes such measurements as size and size distribution, shape and other morphology features (e.g., crystalline, porosity, surface roughness), chemistry of material, solubility, surface area, state of dispersion, surface chemistry and other physicochemical properties. Exhaustive characteristics of test materials are time consuming, expensive and complicated. To some extent, the characterization required depends on the objectives of the characterization required depends on the objectives of the study. However, there are a number of fundamental properties that researchers in the field generally agree must be addressed (Bucher et al., 2004; Oberdorster et al., 2005a, 2005b).This subset forms the basis of a minimum set of characteristics that should be measured for test materials used in nanotoxicity studies. These include size and shape, state of dispersion, physical and chemical properties, surface area and surface chemistry. Each of these properties is explained in the following lines (Kevin et al, 2006).
Size: Particle systems just sometimes are complete sphere, less than most of the time they are like a little particle of material. Nevertheless, in the particle technology community, size of nanoparticle often defines as a diameter of the sphere (Kevin et al, 2006).

Size Distribution: Size distribution are normally depicted as a long-normal histogram with particle diameter on the abscissa and the quantity of particles in a given size class on the ordinate (Allen, T., 2004a).

State of Dispersion: The state of depression of nanoparticle systems refers to the relative number (or mass) of primary (single) particle in a suspending medium in comparison to agglomerates (cluster of primary particles held together by weak forces). These agglomerates may be forms directly from attractive inter-particle forces (e.g., Van der Waals and hydrophobic interactions) or through the binding of adsorbed molecules (e.g., polymers, proteins, polysaccharides). The state of dispersion is one of the most important characteristics of nanoparticle system, yet is one of the most difficult to quantify (Kevin et al, 2006).

Physical and Chemical Properties: Physical and chemical properties include a wide range of particle characteristics, such as elemental composition, density, crystal structure, chemical reactivity, solubility and physical constant such as conductivity, melting point, hardness and optical properties. For many nanoparticles, these properties are the same or similar to the properties of the materials in conventional scale. However, one of the principal reasons that nanoparticles are of interest is the propensity for some of these properties to change as particle size decreases, generally to below 100 nm, and particularly below about 10 nm.

There are many reasons for this problem that why these changes in chemical and physical properties happen: 1) thermo dynamical properties may change because of large radius of curved nanoparticles, high area surface and free surface energy. 2) Quantum limitation and tunneling effect can be due to electro-optical phenomena related to size. 3) Finally, there is one truth that when particle decreasing in size, atomic properties on surface of particle increase (Kevin et al, 2006).

Surface Area and Porosity: Surface area is the area of the material that is exposed to the environment or, alternatively, the interfacial area of the material. Surface area can be external (geometric surface area) as well as internal if the material is porous. Micro porous or mesoporous powders exhibit much higher surface areas than nonporous powder. Materials with pores less than 2 nm are generally considered to be micro porous. Porous between 2 nm and 50 nm are termed mesopores (Kevin et al, 2006).

Surface Chemistry: Surface chemistry consists of wide range of properties that govern on the way that particles interact with their environment. Surface chemistry includes elements of solubility equilibrium, catalytic properties, surface charge, and surface adsorption and desorption of molecules from solution, etc. Most of these properties are functions of atomic or composition of the surface and the physical surface structure. It is important to note that the surface chemistry of particles can change in a variety of ways, particularly through the adsorption or coating of particles with proteins or other species from the biological fluid surrounding them. Particle coatings in particular are problematic, because details such as the coating thickness, continuity, homogeneity, and persistence must all be considered. Quantifying these characteristics can be quite difficult (Kevin et al, 2006). **Surface Structure:** Molecular composition and surface structure of nanoparticle surface are defined by the chemistry of nanoparticle. It is difficult to measure the surface atomic composition directly because most of these systems are influence by surface polluting that is possible not to distinguish by general chemical analysis (Kevin et al, 2006).
Some of applications of nanoparticles based on their properties are summarized in table1.

SOME KIND OF NANOPARTICLES AND THEIR APPLICATIONS IN ENVIRONMENT

Fullerenes

Generally, fullerenes are molecules with 60 carbon atoms that are known as C_{60} . These giant molecules occupied spherical structure so that carbon atoms stand on vertices of the icosahedron structure. Finding real C_{60} during recent 20 years is dedicated wide researches. Most important usage of these materials is solving them into aqueous. These giant compositions cannot be solving in water so it makes limitations for their biological applications. To overcome this problems two ways are exist: 1) non-covalent encapsulation of fullerene molecules into soluble polymeric or host molecules. 2) Covalent functionalization of fullerenes by introduction of hydrophilic groups by chemical modification (Yon and Jamie, 2008).

Carbon Nanotubes

Ijima and co-workers were pioneer in the synthesis of CNTs in 1991, reporting the formation of these nanotubes by using a carbon cathode and the arc discharge technique. However, the discovery of the structure of these Nano materials took place a few years after their first synthesis. There are two main forms of manufactured CNTs, the single-walled or SWCNT, and multi-walled or MWCNT. In terms of structure, the SWCNT is a single-layer grapheme sheet rolled-up as cylindrical shapes, with a diameter of approximately 2 nm and a length of several micrometers, whereas the MWCNT contains two or more concentric layers with various lengths and diameters (Yon and Jamie, 2008).

Table 1: Shown some of nanoparticles applications in environment based on physical properties

		Environmental Applications						
		Pollution Prevention	Sorbents	Composite Filter	Energy Storage	Antimicrobial agents	Aligned CNT Membranes	Sensores
Physical properties	Size		√	√		√	√	√
	Shape					√	√	
	Surface area	√	√	√	√			
	Molecular Specificity		√		√			√
	Hydrophobicity		√	√		√	√	
	Electrical Conductivity				√			√
	Optical Activity		√					
	Thermal Conductivity	√			√			

Metal Oxide Nanoparticle

Metal oxide nanoparticles have a wide applications in terms of food, chemistry science and biologic. Many kinds of metal oxide like TiO_2 Zno, Fe_2O_3 are produced in large amounts during these years. Recently, specific nanoparticles are manufactured from these oxides and introduced in advertisement productions. Such as cosmetic materials and sunscreens (TiO_2 Zno, Fe_2O_3), fillers in dental fillings (SiO_2), in catalysis (TiO_2) and as fuel additive (CeO_2) (Yon and Jamie, 2008).

Iron Oxide Nanoparticle

This nanoparticle has been widely used for biological applications and manufacturing pigments. Many studies are done in order to produce Fe_3O_4 and Fe_2O_3 nanoparticle thae have controlled and stable shape (Yon and Jamie, 2008).

Zinc Oxide Nanoparticle

In recent years, significant properties of zinc oxide attract much attention. ZnO is a semiconductor with direct band gap that band gap energy of it in room temperature is 3.36 eV, high exciting binding energy of 60 meV and high dielectric constant (Singh et al., 2007). Hence, the luminescent properties of ZnO have attracted considerable attention due to its potential application in ultraviolet light emitting devices. Tis band –gap semiconductor has numerous potential applications, particularly in the form of thin films, nanowires, nanorods or nanoparticles (Starowicz and Stypula, 2008) and can be introduced to optoelectronic and electronic devices. They also can be used in the production of chemical sensors and solar cells. One of the most remarkable commercial applications of 20-100 nm ZnO nanoparticles is their used in the production of sunscreens and cosmetics, due to their property of blocking broad UV-A and UV-B rays (Huang et al., 2008).

Titania Nanoparticle (Titanium Dioxide Nanoparticle)

Generally titania is considered as a high band-gap energy semiconductor and because of this reason it is considerable. This nanostructurated material requires the use of near UV light in order to be photoactivated. Consequently, photocatalysis using TiO_2 nanoparticles has recently become very important. The use of TiO_2 nanoparticles has improved the photodegradation process and the complete mineralization of toxic organic pollutants. In fact, TiO2 nanoparticles have been successfully used in environmental technology for the treatment of waste water and groundwater, the removal of benzothiophene from diesel fuel and the degradation of air pollutants, specifically nitrogenoxide, sulforoxides and volatile organic compounds. Although TiO_2 nanoparticles possess large specific surface area, commercial applications have not been developed rapidly due to their tendency to aggregate and coalesce very easily forming larger particles which is an undesirable effect on the catalyst efficiency, and also the difficulties in the separation and recovery of TiO2 particles from the reactant mixture. Nevertheless, TiO_2 is used widely, as with ZnO, in sunscreens, because of its photoactivity. TiO_2 exists in three main crystallographic structures (Yon and Jamie, 2008).

Ceria Nanoparticle

Ceria nanoparticles that are less than 10 nm, are used in nanomaterial and their specific property is being strongly dependent to size and they also can show different quantum effects. Because of being size-dependent nanoparticles, they can be controlled in term of size, and this property supply very important information. There is some difficulties to decrease their size that could be removed by complexion these nanoparticles with cerium sulfide nanoparticle or solving in alumina in room temperature up to 2 nm (Yon and Jamie, 2008).

Metal Nanoparticles

Metal nanoparticles due to be smart are used in catalysts and transporting and other medical and biological applications. One of the excited fields in nanotechnology is that Nano materials carried special properties. Gold, silver and iron are more important (Yon and Jamie, 2008).

Gold and Silver Nanoparticles

Metals nanoparticles are expected to use in biosensors technology in order to distinguish new things that are most based on gold and silver. Silver nanoparticles are applied in advertising cosmetics and as an oxide of bacteria in cotton and other consuming production. Most concerning about these nanoparticles is that they are originally toxic and use as a natural sources and there is possibility to transfer these toxicity into environment. Gold nanoparticles have significant characteristics: stability, non-interaction ability, size- dependent, electronically tunneling and magnetic and optical properties. Chemical properties in nanoparticles are important for covering up materials with nanoparticles (Yon and Jamie, 2008).

Zero-Valent Ion Nanoparticles

Among environmental systems of zero-valent metal nanoparticles, iron zero-valent nanoparticles are used to remove contagious contaminant from aquifer. Several studies have shown that these iron nanoparticles possess the capacity of transforming or sorbing a wide range of common environmental contaminants including chlorinated organic solvents (Zhang, 2003; Elliott and Zhang, 2001; Nutt et al., 2005), organic dyes (Liu et al., 2005), various inorganic compounds (Alowitz and Scherer, 2002; Cao et al., 2005), including metals.

Other Manufactured Nanoparticles

Among other manufactured nanoparticles, those are based on CdS ‹CdSe and CdTe , are known as semiconductor quantum dots. These NPs are attracted many interest in terms of biological molecule, medical and technological information. Cadmium naturally has high toxicity and wide range usage of it need special investigation. Quantum dots are hardly as same as semiconductor when they are in the range 2 to 10 nm. These materials are special structure that neither likes solids nor one unit molecule (Yon and Jamie, 2008).

In table 2, it is tried to categorize entering kinds of nanoparticles into environment according to their applications.

Table 2 : Major routes of input of engineered nanoparticles to the environment for different sectors and applications

Sector/application	Nanomaterial type	Probable exposure routes					
		Air	Surface water	Ground water	Waste water	Soil	Waste
Cosmetics and personal-care product	TiO_2, ZnO, fullerenes(C_{60}), Fe_2O_3, Ag		√		√		
Catalysis, lubricants and fuel additives	CeO_2, Pt, MoS_3	√	√		√		
Paints and Coatings	TiO_2, SiO_2, Ag, quantum dots	√	√		√		
Water treatment and environmental remediation	Fe, Fe-Pd, polyurethane		√	√	√	√	
Agrochemical	SiO_2 (porous) as a carrier	√	√			√	
Food packing	Ag, Nano clay, TiO_2					√	√
Pharmaceuticals and medicines	Nano medication and carrier			√	√	√	

THE MOST SERIOUS REASON TO CHANGE NANOPARTICLES INTO POISONOUS MATERIAL

One of the most important in nanotoxicology is to realize the biocompatibility of nanoparticles. In the following, three factors are mentioned as main reasons of nanoparticle toxicity contact with live cells:

1) Due to chemical toxicity of materials from which they have been made: e.g. Cd^{+2} is relesed from nanoparticles of cadmium selenide. Partial release of ions from nanoparticles is very likely due to high area- to – volume ratio of nanoparticles.

2) Due to small size of nanoparticle: nanoparticle can stick to cellular membranes an enter the cell. Sticking nano particles to memberanes cused nanoparticles accumulate inside the cell an not let it to do its functions. Even nanoparticles do not intract with material inside cells, it still hurt them.

3) due to their shape: for example carbon nanotube can easily pierce cell membrane (Kirchner et al., 2007).

FUNCTION OF NANOFILTER TO WATER TREATMENT

one of the most important application of nanotechnology is nanofilteration that make possible the seperation particle in nanoscale from water and supply high mass refined water production. In this precedure, existance membrane keep two equal phases separate from each other and cause purification water by preventing to pass unwanted impurities. To approach this aim, it requires using forward force that this foce can be the pressure, tempreture, density and even potential difference. A general schematic of nanofilter is shown in Figure 2.

By applying Nano filter, suitable organic materials that are necessary for human health are remain in water but toxic and harmful ones are omitted. According to the point that 50% of aquifer and 78% of water of rivers are not drinkable in local city, application of nanofilteration is too important. Specific kind of Nano filters uses in military conditions to omit chemical contamination from water. In nano filters, water passed through carbon nanotube.

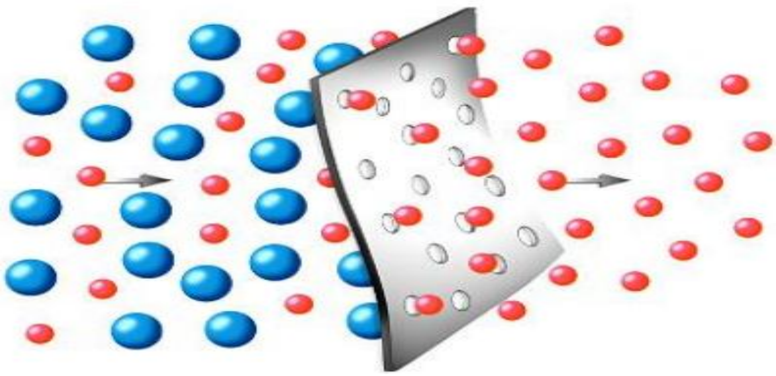

Figure 2: General Schematic of Nano Filter

Carbon nanotube can be used for tracing contamination, also to evaluate probable contaminants in water and collecting information about environmental contaminant. Because nanotubes include nonpolar carbon molecules, by solving in organic solution can stick to other combination and make other contaminants solve and separate from water, so these molecules change then they make tracing possible.

TiO_2 nanoparticles are the most important catalysts which use to omit contamination of organic materials in polluted with oil materials and industrial effluent. Substrates are covered with TiO_2 and put them in the laver that under the ultraviolet radiation. Ultraviolet radiation makes TiO_2 to obtain the ability of oxidation, so TiO_2 nanoparticles can exchange organic material into water, carbon dioxide and mineral acid. Oil effluent is completely decomposed after seven days.

STUDY THE EFFECT OF CRYSTALLINE LATTICE ON MANUFACTURING NANOFILTER

When particles are considered in Nano scale, their properties change and one of the most important factors that made changing in properties is the quantity which is called surface-to-volume ratio.

How this quantity change in nanoparticles can have different effect on their applications. As proved before, material can have arranged crystalline structure when they become nanoparticles. Generally, nanoparticles can save their lattice when they change from bulk into Nano scales.

Studying on Al nanoparticle indicate that if the diameter of NP is less than 5 nm, Al nanoparticle can have different structure from Al bulk. For example, it has been shown that 3-5 nm gold particles have an icosahedral structure rather than the bulk FCC structure. Figure 3 shows three possible arrangements of atoms for the cluster. On the basis of criteria of maximizing the number of bonds and minimizing the number of atoms on the surface, as well as the fact that the structure of bulk is FCC, one might expect the structure of particle to be FCC. However, molecular orbital calculations based on the density functional method predict that the icosahedral form has a lower energy than the other forms, suggesting the possibility of a structural change (Poole and Owens, 2003).

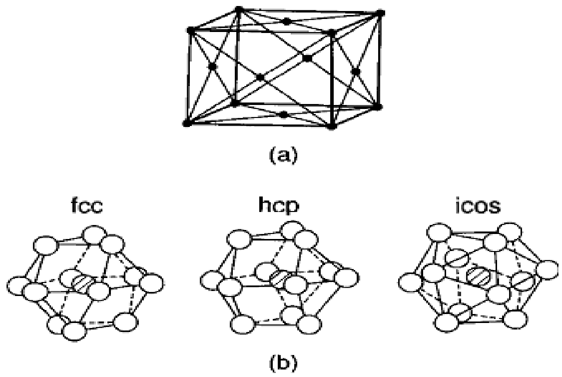

Figure 3: (a) The unit cell of bulk with FCC structure; (b) Three possible structure for nano particle: a face-centered cubic structure (FCC), an hexagonal close-packed structure (HCP), and an icosahedral (ICOS) structure.

Most of the metals in the state of solid have close- packed lattice. metals such as: Ag, Al, Au, Co, Cu, Pb, Pt and Rh; some of the rare gases like: Kr, Ar, Ne and Xe have FCC structure and Mg, Nd, Os, Re, Ru, Y and Zn are in hexagonal close-packed lattice (Poole and Owens, 2003). Figure 4 indicates that FCC structure contain 12 atoms in their nearest neighborhood. FCC and HCP lattice are special because whenever an atom solve in these structures, itself arrange in the special site in shape of FCC in sublattice. Thus, these lattices can solve a large amount of material in their sublattice and be very suitable to manufacturing nano filters. In each unit cell of FCC lattice, there are octahedral and tetrahedral sites. Each tetrahedral can keep only on atom temporarily and each octahedral sites can keep 4 atoms.
So, each unit cell of FCC lattice can keep a large density atom inside itself as sublattice. In Fig.4 you can clearly distinguish lattice and sublattice of FCC, octahedral and tetrahedral sites (Arata and Zhang, 2008; Arata and Zhang, 2002).

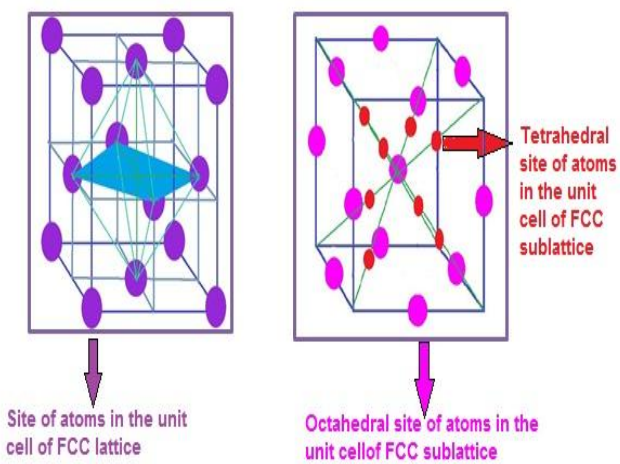

Figure 4: Lattice and Sublattice Structure Are Shown. Octahedral and Tetrahedral Sites in Subllattice Are Indicated

Most of the solid properties depend on their lattice constant. In this case when a FCC bulk structure change into FCC nanoparticles, some properties like lattice constant state their connection between atoms. For example, in GaAs nano particle, if unit cell has a FCC lattice, nanostructure contains n^3 unit cell.

Then, we show that the number of surface atoms N_s, numbet of total atoms, size or dimentional of unit cell (d) coud be find with following equations (Poole and Owens, 2003):

$$N_s = 12n^2 \quad (1)$$

$$N_T = 8n^3 + 6n^2 + 3n \quad (2)$$

d=na , a=lattic constant (3)

Magnitude of percentage of atoms on surface for small n is one of the essential factors that make difference between nanoparticles and their bulks. n is the number of layer that exist in nano structure. These calculations are summerized in table3. Those equations for FCC lattice formulated in the following:

$$N_T = \frac{1}{3}(10n^3 - 15n^2 + 11n - 3) \quad (4)$$

$$N_s = 10n^2 - 20n + 12 \quad (5)$$

$(2n-1)d$ is the diameter of each nanoparticle, d is the distance of nearest neighborhood.

$$d = \frac{a}{\sqrt{2}} \quad (6)$$

In above formula, n is the number of existence layer in nanostructure that can assign 1, 2 ,3 ,4 ,5 ,6 ,7 ,8 ,9 ,10 ,11 ,12,25,50,75,100 number. The calculations for FCC lattice are shown in table4 (Poole and Owens, 2003).

Table 3: Number of atoms on the surface, and percentage of atoms on the surface of different GaAs nanoparticle Size

n Number of layer in nanostructure	Size na (nm)	Total number of atoms	Number of surface atoms	Percentage of atoms on surface
2	1.13	94	48	51.1
3	1.70	279	108	38.7
4	2.26	620	192	31.0
5	2.83	1165	300	25.8
6	3.39	1962	432	22.0
10	5.65	8630	1200	13.9
15	8.48	2.84×10^4	2700	9.5
25	14.1	1.29×10^5	7500	5.8
50	28.3	1.02×10^6	3.0×10^4	2.9
100	56.5	8.06×10^6	1.2×10^5	1.5

Table 4: Numbers of atoms in metallic and rare gas nanoparticles with face-centered cubic close-packed structure

Number of layer in nanostructure	Diameter (nm)	Total number of atoms	Number of surface atoms	Percentage of atoms on surface
I	Id	I	1	100
2	3d	13	12	92.3
3	5d	55	42	16.4
4	7d	147	92	62.6
5	9d	309	162	52.4
6	11d	561	252	44.9
7	13d	923	362	39.2
8	15d	1415	492	34.8
9	17d	2057	642	31.2
10	19d	2869	812	28.3
11	21d	3871	1002	25.9
12	23d	5083	1212	23.8
25	49d	4.90×10^4	5.76×10^3	11.7
50	99d	4.04×10^5	2.40×10^4	5.9
75	149d	1.38×10^6	5.48×10^4	4.0
100	199d	3.28×10^6	9.80×10^4	3.0

7- DISCUSSION AND CONCLUSION

These dayes, utilization of nanotechnology required to know nanoparticles as best as we can. One of the most important factor which make nanoparticles to be distinct from their bulk is that the surface volume ratio in nanoparticles is much more larger than it in bulk size. Among all characteristics of nanoparticles, the most significant factor which effect on the number. of surface atoms in NPs is , when bulk

materials change into nanostructure stand in arranged one.If the effect of crystalline lattice is considered and investigated carefully, we notice that nanostructures with FCC lattice are more sitable to make nanofilters. Because their lattice allows them to solve much more amount of contaminations in their sublattice. So these kind of nanofilters due to their lattice can seprate useful and harmful particles better from air, water and etc.

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