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SIGNIFICANCE OF LATTICE THEORY IN ESTABLISHING SELECTED METAL NANO CRYSTALLITE STRUCTURES

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ABSTRACT

The significant progress in nano science and nanotechnology has developed number of particles in varied shapes. When nucleated and grown in a solution or on a substrate, the metal structure of a crystallite is strongly affected by its interaction with the environment. The developed nano particles of cube, cuboids, octahedron , tetrahedron right bipyramids , icosahedrons, rod or wire shapes with circular, square, rectangular, pentagonal or octagonal cross sections. For single-crystal Ag and Pd seeds terminated with only {111} and {100} facets, metal atoms will add preferentially to the poorly passivated {111} facets, these atoms then migrate to the face edges, resulting in an elongation of the {100} facets and the formation of nanocubes.[2] In our presentation Palladium lattices and TEM images are studied under varied controlled conditions and described.

Keywords: *Lattices, facets, controlled conditions*.

Introduction

Mathematics is used widely in chemistry as well as all other sciences. Mathematical concepts are absolutely necessary to explore important concepts in chemistry. Without some basic numerical skills and calculations, chemistry itself, will be extremely difficult. However, with a basic knowledge of some of the mathematics the concepts of lattice theory will be well implemented to deal with the concepts and theories of chemistry.

It is important that characteristic of a crystalline structure is its atomic packing factor. This is calculated by assuming that all the atoms are identical spheres, with radius large enough that each sphere abuts the next. The atomic packing factor is the proportion of space filled by these spheres. By assuming one atom per lattice point, in a primitive cubic lattice with cube side length a, the sphere radius would be $a/2$ and the atomic packing factor turns out to be about 0.524.

Majority of the metals crystallizes in the same cubic close-packed (ccp) structure, a face-centered cubic (FCC) lattice that allows for easy characterization [1]. Nano technology provides the most powerful means to manipulate the electronic, optical, and magnetic properties of a solid material. Among the various kinds of inorganic solids, metals deserve our special attention because they represent more than 60% of the elements in the period table. Metals exhibit range of wonderful properties, and many metals have broad range of applications that includes catalysis,[2]electronics, photography,[3] and information storage,[4] among others.[5] Recent trends demonstrates the exploitation of applications for metals in areas such as photonics, sensing, imaging, and medicine[6] are also being developed. Significantly, most of these applications require

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the use of metals in a finely divided state, preferably in the form of nano crystals with precisely controlled properties. Over the last decade we have been witnessed the successful synthesis of metal nano crystals in a variety of shapes. Examples include: sphere, spheroid, cube, cuboctahedron, octahedron, tetrahedron, right bipyramid, decahedron, icosahedrons, thin plate with a triangular, hexagonal, or circular profile and rod or wire with a circular, square, rectangular, pentagonal, or octagonal cross sections [7, 8, 9]. According to Wulff''s theorem (or the Wulff construction) [10] a single crystal of an FCC metal assumes the so-called Wulff polyhedron (a truncated octahedron) as its equilibrium shape in an inert gas or vacuum. However the product often adopts a shape drastically different from the Wulff polyhedron. D.Keerthi *etal* has demonstrated Pd nanoparticles capped with Gum Acacia with lattice planes indexed as (111),(200),(220),((311) and (222) with the shapes pertaining to spherical and polyhedron shapes.[11] Larsen T.H. *etal* has reported solvent free synthesis, [12,14] and various shapes of nanostructures have been synthesized, including Cu_2S nanoparticles[12,13] nanorods,[12,13] nanodisks,[12,13] nanoplates,[12,13] NiS nanorods, and triangular nanoprisms.[14].The same authors demonstrated the NiS nanorods which are triangular nanoprisms prepared by the same method.[14]The possible crystal planes were in support with XRD data, the respective lattice planes were presented in **Figure-I**.

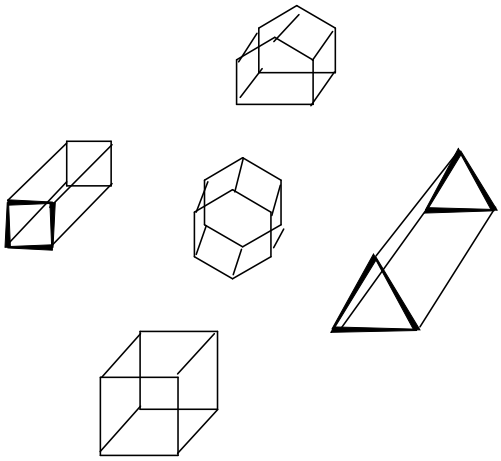

Figure I: Possible lattice planes for some nano particles

Materials

All the chemicals NaOH, HCl, were of analytical grade, S.D.Fine Chemicals (Mumbai, India) and Palladium (II) Chloride from Sigma Aldrich Chemicals Co Inc.(Sleeze, Germany),the aqueous solutions were made with 2D distilled water.

Synthesis of Pd nanoparticles:

The calculated amount of $PdCl_2$ (0.106g) was dissolved in 300ml of $8x10^{-4}$ M HCl to form H_2PdCl_2 aqueous solution. An aliquot of 5ml of 0.2% was mixed with 5 ml of saffron extract. The reaction mixture was heated at different temperatures (40, 60, 80 and100^0C) for about 8 hrs. Within short time the rapid colour changes were noticed, pale yellow to deep brown which indicates the formation of nanoparticles. The progress of reduction was monitored by UV-Visible spectrophotometer. The growth of nano crystallites was periodically recorded at every 30 min for 48hrs.The suspension was centrifuged with acetone. The residual Pd nano particles were recovered

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and air dried. The same procedure was carried out with 5ml of 0.4, 0.6,0.8, 1%.

Characterization of Palladium nanoparticles (PdNP):

UV visible spectroscopy is one of the most suitable techniques for the characterization of Palladium nanoparticles. PdNP shows strong absorption band due to large surface area, earlier reports on heating in presence of H_2O, glycerol, vinyl alcohol medium [14].Reaction performed at 100-110^{0}C showed completion of reduction which was monitored by spectrophotometer and absorption recorded at 400nm.

(ii) By FT –IR studies:

The IR spectrum was recorded for saffron loaded Palladium nanoparticles. In the IR spectrum strong peaks appeared 1650Cm^{-1}, 1430 Cm^{-1} representing –COO and -OH groups present in Crocin which was the major component in the saffron extract.

iii) By XRD studies – Peak indexing:

XRD pattern of **PdNP** was recorded and the Peaks consistent with the Face Centered Cubic (FCC) as expected for Palladium nanoparticles. Indexing process of powder diffraction pattern is done and Miller indices (h k l) for each peak are assigned in the first step. A number of strong Bragg reflections can be seen which corresponds to the (111) (200).The size of the Pd nanoparticles were calculated from the Debye-Scherrer's formula.

Debye-Scherrer's formula: **$B=k\lambda / s\cos\theta$**

Where, **S** is the crystallite size, **λ** is the wave length of the X-ray radiation, **K** is constant taken as 0.94, **θ** is the diffraction angle and **B** is the line width at half maximum height.

The Debye-Scherrer's formula used for the interpretation where shape, size of the crystallite by the application of trigonometry. The purity was also addressed by XRD analysis.

iv) Crystal Lattice Indexing through Transmission Electron Microscopy:

The synthesized nanoparticles were examined further by Transmission Electron Microscopy (TEM).SEAD pattern of TEM image was presented in **Figure-II.** It exhibits five main diffused rings which were characteristic of crystalline orientation and they were indexed to be (111), (200), (220), (311), (222).The

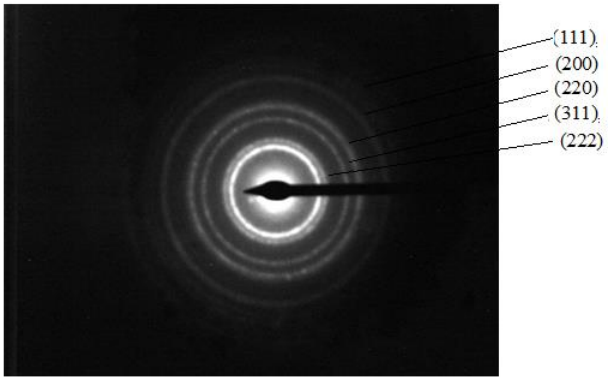

Figure-II:TEM images of PdNp - Palladium metal encapsulation SAED pattern of indexing

CONCLUSIONS

The developed nano particles into of cube, cubiod, right bipyramids , rod or wire shapes with circular, square, rectangular, pentagonal shapes were purely based on the synthetic conditions. Each

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metal has its unique property in exhibiting the crystal lattice places, the palladium nanoparticles lattice plane that were presented in this paper as Face Centered Cubic (FCC) lattice planes. The importance of lattice planes for the interpretation and the possible geometry on the three dimensional frame was only done with the mathematical applications of lattice theory.

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