Modeling in nanotechnology using structural models of the atoms derived by the unified theory Basic Structures of Matter

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1. Introduction The reader not acquainted with the BSM theory may read the article "Brief Introduction to BSM theory".

Abstract of the article *Brief introduction to the theory Basic Structures of atoms and derived atomic models*. The relation between the gravitational filed, from one side, and the electrical and magnetic, from the other is a long standing problem. Its successful solution might be quite dependable of the concept of the vacuum space. This concept has been changed four times since the seventeen century. If the currently accepted concept about the vacuum space is not correct, our vision about the matter structures and processes in the microscale range might be distorted. An interdisciplinary study from different fields of physics and chemistry indicates that the real atoms are different from the planetary atomic models. This difference is not of energetic but of structural aspect. Based on a new concept about the vacuum space, a recently developed unified theory called Basic Structures of Matter (BSM) allowed unveiling of the real physical structures of the atoms and the elementary particles. The obtained physical models of the atoms exhibit the same energetic levels as the quantum mechanical models, while possessing nuclear structures different from the nuclei in the planetary atomic models. The derived models with fully identifiable parameters and positions of quantum orbits allows studying the physical conditions behind the structural and bond restrictions of the atoms connected in molecules. The existing data base about structure and atomic composition of the organic and biomolecules provides an excellent opportunity for reliable validation of the derived physical models of the atoms. The suggested models could be useful for theoretical analysis of organic and biomolecules and for structure modelling in the fields of nanotechnology.

Between the most useful results of the BSM theory are the derived physical models of the atoms. They look quite different in comparison to the planetary atomic models, but exhibit the same energy levels and interaction properties as the Quantum mechanical models. The physical models, however, possess structure defined by the atomic nucleus. The protons and neutrons in the nucleus are arranged in well-defined order with Z-trend signature matching the raw and column features of the Periodic table. They define the positions of the quantum orbits and chemical bonds. In such way the derived physical models provide explanation about the length and angular restrictions of the chemical bonds. The different concept of the atomic nucleus and its spatial configuration is a result of the alternative concept about the vacuum space. The Atlas of the Atomic Nuclear Structures is a direct result of the BSM theory. It provides three-dimensional configuration of the stable elements for Z ranging from 1 to 103 (from H to Lr).

Fig. 1 provides illustration about the overall shapes of the proton and neutron and their arrangement in the simplest atomic nuclei as Deuteron and Helium. The possible quantum orbits for Hydrogen and Deuteron are also shown. The surfaces in which the quantum orbits lie in fact intercept the equivalent plane of the proton at right angle. The two separated orbits of the He (not shown) have four leafs and also are perpendicular to the equivalent proton planes.

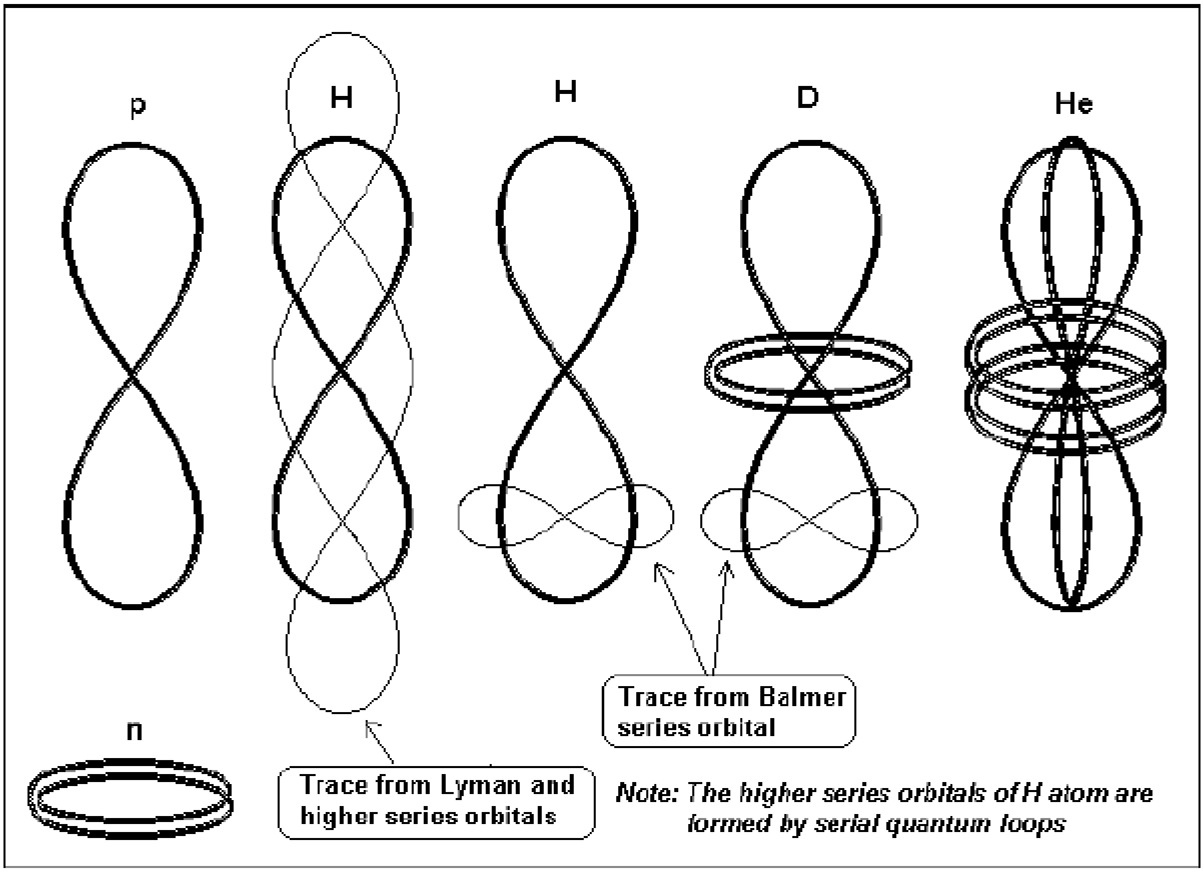
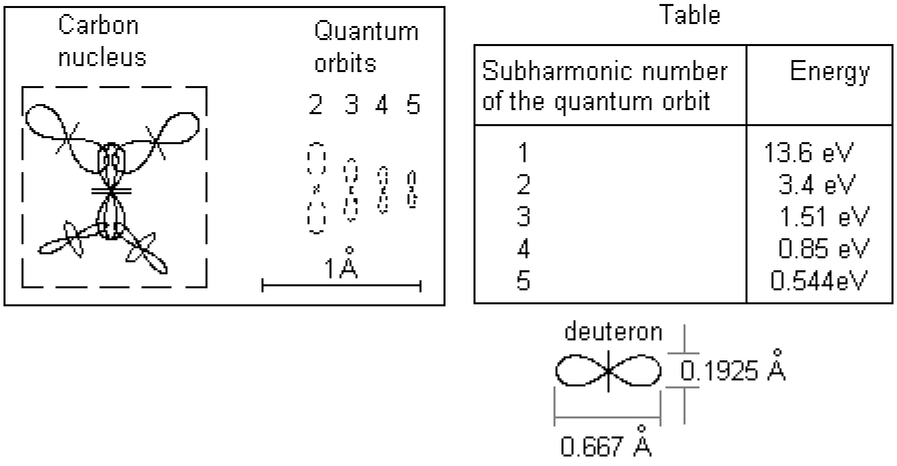


Fig. 1

Fig. 5 shows the physical model of the Carbon atom in which the protons and neutrons are presented by symbolic notations. The left part of the figure shows an axonometric view of the carbon atom. The He nucleus is embedded in the carbon nucleus with its long axis defining the polar axis of carbon nucleus (this feature is valid for all atoms). The two protons (deuterons) in the top pole have a limited angular freedom in the plane of the drawing. The two protons (deuterons) in the bottom pole have a limited angular freedom in a plane perpendicular to the drawing. The right part of the figure shows the possible dimensions of the quantum orbits, denoted by the subharmonic number of the oscillating electron and corresponding to electron energies as shown in the Table at the left side of the figure (see Chapter 3 of BSM). The quantum orbits as a rule of drawing in BSM models are drawn by a dashed line. The proton dimensions and the size of the possible quantum orbits are in one and a same scale.

In the bottom part of the figure the sketch of the deuteron is shown in which dimensions of the proton are given. The deuteron is the most frequent building block in the atomic nuclei. The other basic building block is the ^{4}He nucleus. It is the most dens structure of stable atomic nuclei, so it is always in the middle of the nuclei. (For more details see Chapter 8 of BSM and Atlas of ANS).



Table

Subharmonic number of the quantum orbit	Energy
1	13.6 eV
2	3.4 eV
3	1.51 eV
4	0.85 eV
5	0.544eV

Fig. 2

2. Application in nanotechnology. The physical models of the atoms provide a great opportunity for a modeling of different structures in nanotechnology. Such modeling could serve as a preliminary design of molecular structures in which selected atoms serve as building blocks. In such design, not only the possible combinations could be examined, but also the position and orientation of any quantum orbit can be identified.

Fig. 3. provides an axonometric view of a part of single-walled carbon nanotube, as known by the current knowledge. The cylindrical part of this nanotube does not contain any defect and all ring structures involves 6 carbon atoms. If imaging that the cylindrical surface of such nanotube is unfolded it will be a flat sheet without bumps or dimples. If some ring structure, however, contains 5 carbon atoms, a bump or dimple will occur. The closed end of the nanotube should contain such structures.

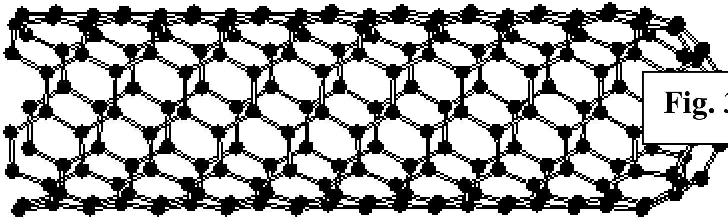
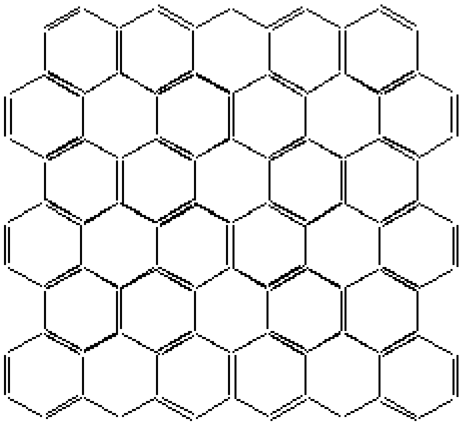


Fig. 3

Fig. 4 shows a sheet of the unfolded cylindrical wall with identified valence of the chemical bonds, so that the four valences of all carbon atoms (excluding the edge atoms) are connected.



Let considering the hexagonal ring as a unit structure of the sheet. Then the sheet is comprised of two types of ring structures:

- ring structure of I-st type (containing only single valence bonds)

- ring structures of II-nd type (containing tree single valence bonds and three second valence bonds).

Fig. 5 provides an axonometric view of a sheet, corresponding to unfolded cylindrical part of single walled carbon nanotube. The rings of I-st type are clearly distinguishable from the rings of II-nd type. The protons, involved in the second valence bonds lie in plane perpendicular to the sheet plane. In the same figure all quantum orbits providing chemical bonding are also shown. The quantum orbits of the free (nod bound) protons in the edges are shown, as well.

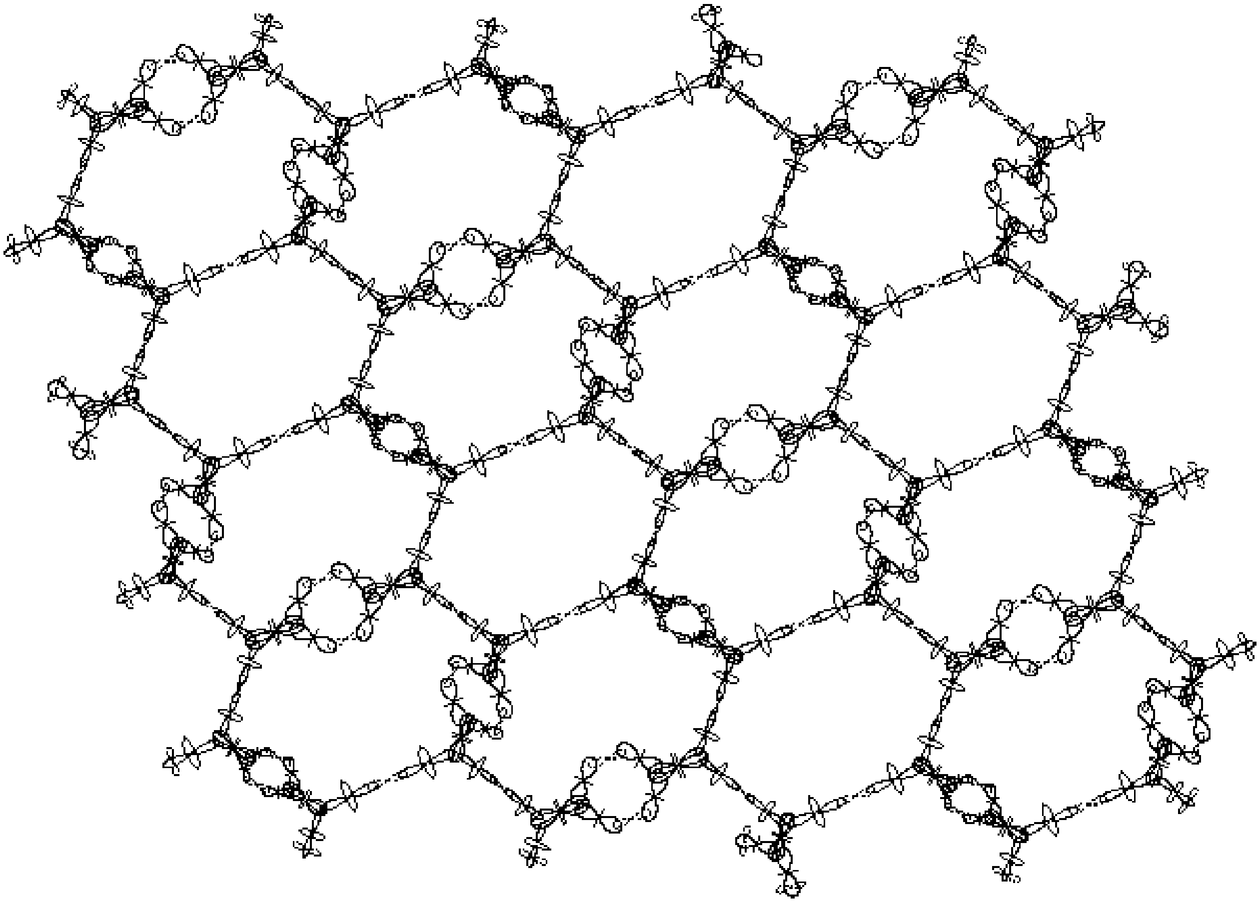


Fig. 5

From Fig. 4 and Fig. 5 it is evident that every ring structure of I-st type has 3 neighbors of same type and 3 neighbors of second type, while every ring structures of II-nd type has 6 neighbors of same type. Therefore the overall ratio between the two types ring structures is 1/2.

Fig. 6 shows a zoomed section from the carbon wall sheet, so the orbital positions are shown clearer. The two orbitals of He nucleus of carbon atoms are not shown. If regarding the sheet as built of lower level atomic structures it contains only He nuclei and deuterons. However, the four deuterons are very strongly bound to the He nuclei assuring the compactness of the carbon atom. These types of nuclear bonds between protons and neutrons are hold by very strong forces, whose origin is analyzed in details in BSM theory. In comparison to them the electronic bonds forming quantum orbits are extremely weak.

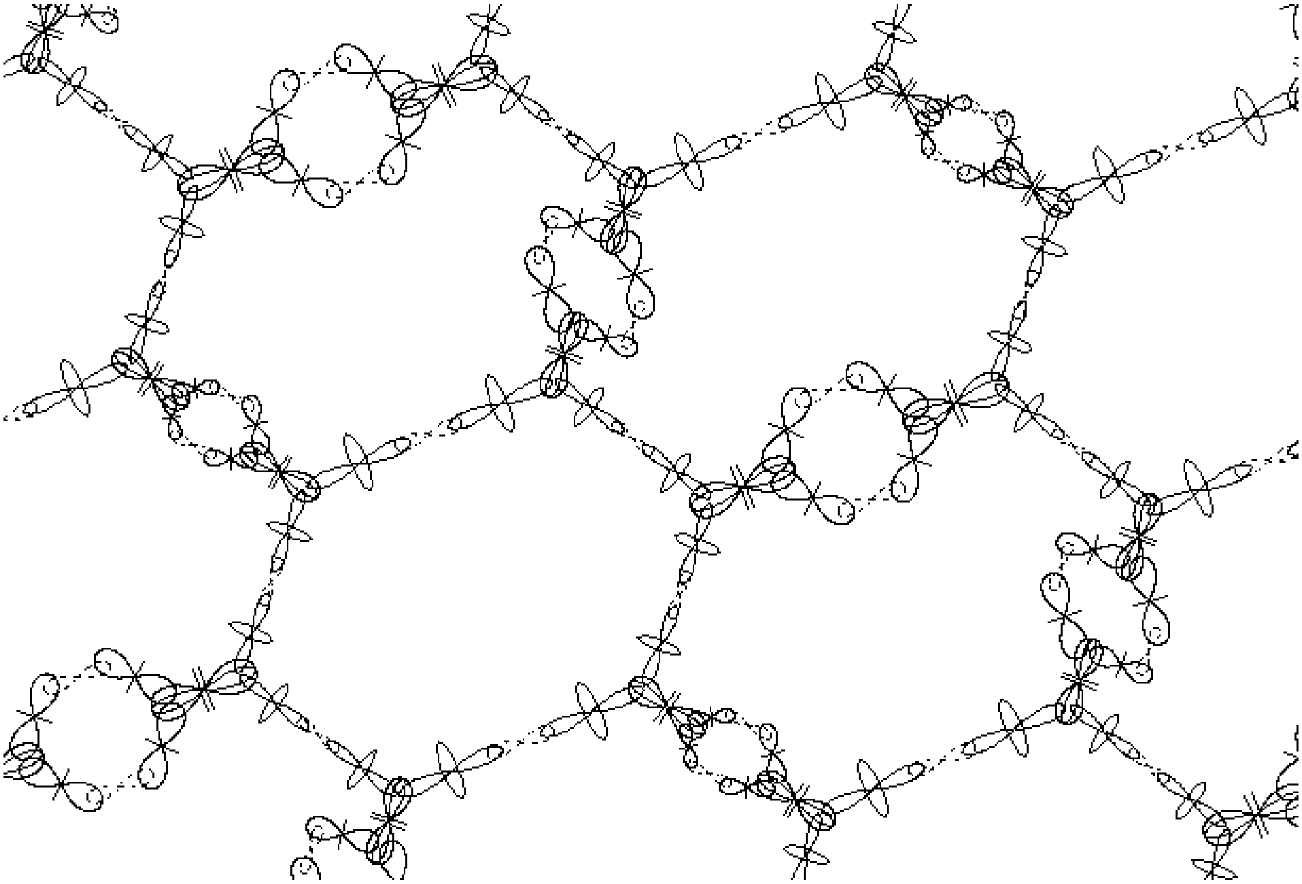


Fig. 6

It is evident that the ring of I-st type could be also a pentagon instead of hexagon and then it will have 5 neighboring rings of second order. Carbon wall sheet containing a pentagon will get a bending.

Not only the structural design but also the conductive properties of the designed structures could be inferred, if preliminary knowledge about the orbital distances and positions corresponding to bandgap between a conductive and isolating state are available. This requires knowledge about the spatial configuration of the proximity electrical field of the proton and the possible influence of the closely spaced protons on the quantum orbits. (this could be obtained by approximate theoretical modeling). The provided considerations are analytical results from the BSM theory about the electrical field of the elementary particles.

Examining the quantum orbits involved in the chemical bonds it is evident that the plane orientation of the quantum orbits in the single valence bonds are different from the plane orientations of the second valence bonds. For electrical neutral state of the sheet all quantum orbits contain two electrons with opposite quantum mechanical spins (referenced to the proton twisting). It is possible, however, in conditions of very strong external electrical field, the local fields of the protons to be biased. Then one of the two electrons in the chemical bond quantum orbits might be separated as a free electron providing conductivity. A quantum orbit with only one electron is also possible, but its shape (and eventually the subharmonic number) could be possibly changed.

The suggested method could be also used successfully for thin crystal layers grown by molecular beam epitaxy. Fig. 7, for example shows the atom of gold (according BSM concept) in two views: the right side view is a polar view, while the left side view is a polar sectional view in which only the protons (deuterons) closer to the sectional plane are shown. He nuclei as most dens atomic structures are always in the middle of the atomic nucleus and aligned with the polar axis of the atom.

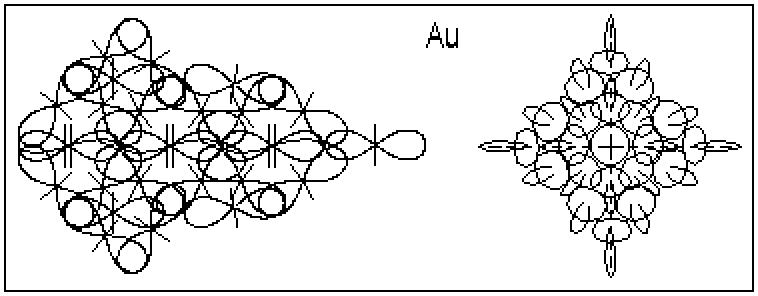


Fig. 6

Fig. 7 shows images of two crystal planes of gold layer obtained by one of the most powerful transmission electron microscope (Japan) (T. Kawasaki et al., Applied Physics Letters, v. 76, No 10, p. 1342-1344 (2000))

In the next page a comparison between image of two planes of gold crystal and the model design using the physical structures of the atom of gold are shown.

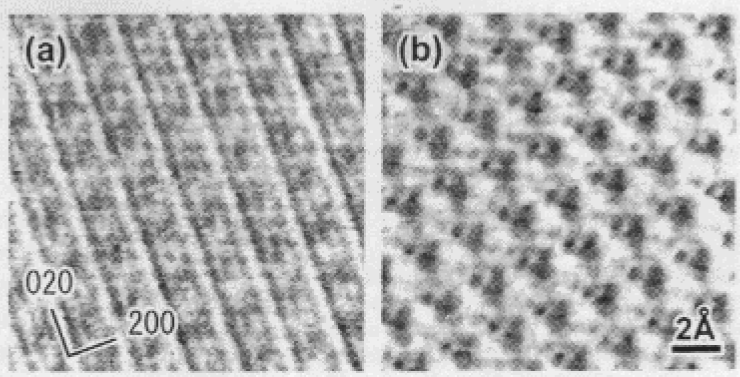
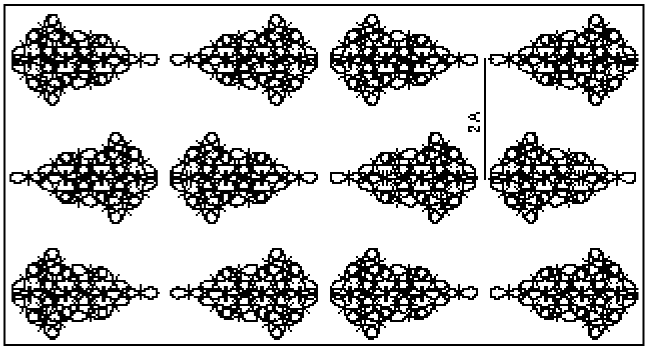


FIG. 2. (200) lattice fringe ($d = 2.04$ Å) images of a Au(001) thin film: (a) 1/3 spacing fringes formed from ($\bar{2}00$) and (400) reflections; and (b) fringes formed from many high-order reflections. The Fourier transform of the micrograph extends to ~0.5 Å

Fig. 7 Courtesy of T. Kawasaki et al., Applied Physics Letters, v. 76, No 10, p. 1342-1344 (2000)

Fig. 8 and Fig. 9 show two theoretical patterns corresponding to two possible spatial orders (or crystal planes) of Au atoms in the metal crystal lattice. The nuclear size of Au atom is based on the calculated proton dimensions while the internuclear distance matches the dimensions of the possible quantum orbits. The proton dimensions and quantum orbits are calculated by the model analysis in BSM theory and expressed by the physical constants. The theoretically obtained interatomic distance of 2 A matches the experimentally observed distance shown in Fig. 9. The pattern shown in Fig. 8 is quite similar to the observed pattern given in Fig. 7 (a), while the pattern in Fig. 9 possesses alignment features, which might contribute to the observed pattern in Fig. 7. (b).



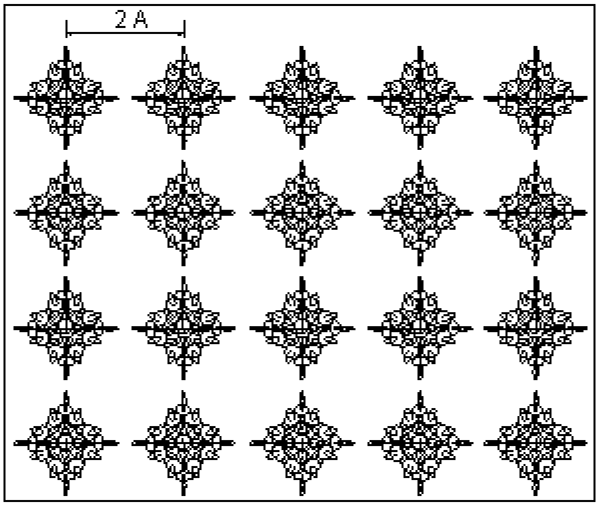


Fig. 8

Fig. 9

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