

## A survey of the liquid-crystal phase transition of a hard sphere BCC with the optimized spherical approximation based on the modified weighted density function theory and its application in color science.

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**Abstract:** In accordance with the weighted density function theory (WDA), another formulation for the non-uniform classical fluids has been suggested. This mentioned formula has been termed as “the modified weighted-density approximation (MWDA)”. One of the first usages of this approximation and one of the primary inputs is choosing the appropriate correlated function related to the interaction of the corresponding sector. For this particular purpose, a different correlated function has been used – such as PY and PELK functions. In this part, we use crystalline solid (BCC) and the correlated function spectacularly. Indeed, for the non-uniform classical fluid, the same approximation of hard spherical molecules will be considered. Eventually, the application of practical consequences relevant to this new approach in the resin and color industries will be surveyed. Besides, we examine the new conditions from the practical perspectives.

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**Keywords:** BCC structure; MWDA; WDA; weighted density function; interaction potential; density profile.

### 1. Introduction

First of all, we will derive the weighted density function from the theoretical perspective. Then, the main characteristics of the BCC solid are surveyed. Afterwards, we will express how the transition of the notions of solid state physics related to the calculation of multi-phase and practical process will be done. After that, we concentrate on the main subject. Hence we investigate the phase transition of the materials with spherical molecules in a sequence. The usage of the density functional theory for survey of phase transition refers to 50's which has been developed significantly so far. Certainly, most of researches have been conducted on the crystals with FCC structure but in this investigation, the crystals with BCC structure are studied.

Our main emphasis would be on the type and structure of the corresponding solid and leaving a little spherical shape is vital. Then, we will answer this question which under what circumstances the transition of BCC liquid-crystal phase for materials with hard sphere molecules and optimized spherical approximation can be done. For this purpose, the following assumptions could aid us:

- 1- Use the potential of the hard sphere with optimized spherical approximation.
- 2- Density functional theory based on the equivalency or coexistence of BCC crystal and fluid.

Next, we use the outcomes in practical applications such as the interaction of color layer with different surfaces (BCC structure). Finally, we express the practical concepts of the mentioned results.

### 2. The theoretical structure of BCC solid and the modified weighted density function theory (MWDA)

#### 2-a. The weighted density approximation (WDA)

For a very little classical system, *Helmholtz* extra free energy,  $F_{ex}(P)$ , is a unique function of the density  $P$ , as shown in the below form:

$$f_{ex}(P) = \int \vec{d}\vec{v} \vec{p}(\vec{r}) f(\vec{v};(\vec{p})) \quad (1)$$

Where  $f(\vec{v};(\vec{p}))$  shows the extra free energy of the substance. In this approximation, the extra energy is defined as follows:

$$f_{ex}^{WDA}(P) = \int \vec{d}\vec{v} \vec{p}(\vec{r}) f(\vec{v};(\vec{r})) \quad (2)$$

where  $f_0$  is related to extra free energy on the particle of the uniform fluid and  $\vec{p}(\vec{r})$  is the average of the weighted density for the single-particle,  $\vec{p}(\vec{r})$ , in accordance with the weighted function  $\vec{w}$ , it means:

$$\int \vec{d}\vec{r}' \vec{p}(\vec{r}') \vec{w}(\vec{r} - \vec{r}') = w(\vec{r} - \vec{r}'; \vec{p}(\vec{r}')) \quad (3)$$

It satisfies its particular weighted function with ease.

$$\int d\vec{r}' w(\vec{r}' - \vec{r}; p(r)) = 1 \tag{4}$$

Now, the correlated function is inserted. The connection between the correlated function of  $n$  particles and  $f_{ex}(p)$  is formed by this way:

$$c^{(n)}(\vec{r}_1, \dots, \vec{r}_n; p) = -\beta \frac{\delta^n f_{ex}(p)}{\delta p(\vec{r}_1) \dots \delta p(\vec{r}_n)} \tag{5}$$

For  $n=2$ :

$$c^{(2)}(\vec{r} - \vec{r}'; p_0) = -\beta \lim_{p \rightarrow p_0} \frac{\delta^2 f_{ex}(p)}{\delta p(\vec{r}) \delta p(\vec{r}')} \tag{6}$$

Finally, by using the conversion:

$$-\beta^{-1} c_0^{(2)}(x; p) = 2f_0(p_0)w(x; p_0) + p_0 f_0'(p_0)w^2(x; p_0) + 2p_0 f_0'(p_0)w'(x; p_0)w(x; p_0) \tag{7}$$

The last formula is the same approximation of the weighted density which had been proposed by *Achcroft*.

2-b. The modified weighted density approximation (*MWDA*)

In WDA, used approximation  $f(\vec{r}; (p))$  determines the extra free energy on the particle.

But in the modified weighted density approximation, the formulation concentrated on the extra free energy on the particle will be in this form:  $f_{ex}(p) / N$  where  $N$  is the number of particles in the system. It is obvious that  $f_{ex}(p) / N$  in comparison with  $f(\vec{r}, (p))$  does not depend on the conditions.

We show this approximation with  $P'$ . Indeed, it is independent of the place which makes it different from  $\bar{P}(\vec{r})$ . So, *MWDA* is a method which could measure  $f_{ex}(p) / N$ .

Thus, we will have:

$$f_{ex}^{MWDA}(P) / N = f_0(\hat{p}) \tag{8}$$

$$\hat{p} \equiv \frac{1}{N} \int d\vec{r} p(\vec{r}) \int d\vec{r}' p(\vec{r}') \tilde{w}(\vec{r} - \vec{r}'; \hat{p})$$

And the weighted function satisfies the circumstance of interaction, again.

$$\int d\vec{r}' w(\vec{r} - \vec{r}'; \hat{p}) = 1$$

By combining two mentioned formulas -number 6 and 9- where  $V$  is termed as the volume of the system. By using the direct Fourier conversion, We will arrive at this:

$$\tilde{w}(x; p_0) = \frac{-1}{2f_0'(p_0)} \left[ \beta^{-1} c_0^{(2)}(x; p_0) + \delta_x p_0 f_0''(p_0) \right] \tag{10}$$

Clearly, this formula is the modified weighted density approximation.

2-c. BCC solid

So as to use the modified weighted density approximation in surveying the interaction of gas-liquid- solid, the weighted density of the corresponding solid should be calculated first. Hence the attributes of BCC crystals must be considered in brief. Then, the function of its weighted density  $\tilde{w}$  will be computed in Fourier space. By doing this task through the formula  $\tilde{w}$ , the collective integrals are converted into the sum of the vectors of the reverse solid network.

In a nutshell, there exists around fourteen types of network molecular arrangement or cellular structure. A large number of metals and most of the other solids possess molecular structure in shapes of body-centered cubic (BCC), face centered cubic (FCC) and hexagonal closed packed (HCP).

In BCC system, there is an atom on each of eight corners and in the intersection of diameters. Each of the eight corners of the cube is a corner of other cubes. Therefore, 8/1 of the atom in the cube, will be the corresponding share. It means that the coordination number of the atom is 8 and the share of each unit will be 12 full-atom. One of them is the central atom and another one is the result of 8 of 8/1 atom located on the corners.

This structure does not allow atoms to get close together very much. Commonly, This kind of solid is witnessed in metals which are formed at the high temperature and are cooled at the low temperatures slightly. In figure 1, a free selection for the BCC network vectors has been recommended. By this choice, we will possess an appropriate form in order to compute and work with vectors of the reverse network. There is a point, it could be proved that the reverse network of BCC is the same one of FCC, and vice versa.

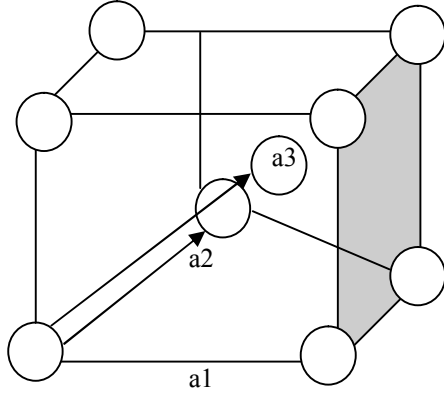


Figure 1. BCC Solid network vectors

The reverse space or the n-dimensional space is the one which the Fourier conversion function is defined for a specific function (as an illustration, the frequency domain is defined in a space with the Fourier conversion for a time-dependent function) Fourier conversion transforms us from the main space to reverse one, and vice versa. Generally, we have:

$$f(\vec{x}) = \int_{-\infty}^{\infty} f(\vec{r}) e^{-i\vec{x}\cdot\vec{r}} d^3r \quad (11)$$

The reverse space is a different set of points in this space and the vector of  $\vec{x}$  is the maker of the image connected to the major space. Brillouin zone in this space is the volume which includes all the unit vectors with the periodic structure itself. So as to calculate on the bases, we will show the Fourier conversion as follows:

$$f\vec{\sigma} = N \int dv n(\vec{r}) \exp(i\vec{\sigma}\cdot\vec{r}) = NS\sigma \quad (12)$$

Where  $N$  is named as the number of crystal cells. When  $\vec{r} = 0$  is matching with one of unit atoms located on the corners, we can write the electron distribution:

$$n(\vec{r}) = \sum n_j(\vec{r} - \vec{r}_j) \quad (13)$$

By expressing the structural function as the sum over all atoms in the cell, we will arrive at:

$$s\vec{\sigma} = \sum_j f_j \exp[-i 2\pi (hx_j + xy_j + hz_j)] \quad (14)$$

In the above formula,  $f_j$  is the atomic coefficient and

$\vec{r}_j = x_j\vec{a}_1 + y_j\vec{a}_2 + z_j\vec{a}_3$  is the vector of the main network and  $\vec{\sigma} = h\vec{b}_1 + h\vec{b}_2 + h\vec{b}_3$  is the reverse network vector. Now, for instant, we are going to survey the connection between the reverse network vectors and main ones of BCC and FCC crystals. The former ones are smaller than the latter. As an illustration, for BCC solid with the fixed network number  $a$ , this amount for the reverse space of the FCC solid will be  $\frac{4\pi}{a}$ . So, the shortest vector of the reverse network from one corner to the center of adjacent face will be the below amount:

$$\left(\frac{4\pi}{a}\right)(1.2, 1.2, 0)$$

For example for Iron, by the final length  $2\sqrt{2}\pi/a$ , we have:  $a = 3.59 \text{ \AA}$  and the length of the reverse network vector is 24.8 nanometers.

To compute the functional fixed number for each particular network, we have to do the summation upon all atoms in the unit cell and since the crystals are often described in terms of Miller indices, so we also use them for calculations.

As far as we know, the BCC system is described as a simple cubic one with these vectors  $a\hat{x}$ ,  $a\hat{y}$  and  $a\hat{z}$  and a primary assumption;  $\vec{r}_1 = \frac{a}{2}(\hat{x} + \hat{y} + \hat{z})$  and  $\vec{r}_0 = 0$ . Clearly, its reverse network is the same simple cubic system with the network constant number  $2\pi/a$ . In a single-atom crystal, all structural functions,  $f$ , are the same. The intensity of the scattered beam together with this vector,  $x = \frac{2\pi}{a}(h\hat{x}^* + x\hat{y}^* + l\hat{z}^*)$  from this surface  $(hkl)$  is shown as:

$$\begin{aligned} f_x &= f \left[ e^{-i\vec{x}\cdot\vec{0}} + e^{-i\vec{x}\cdot\left(\frac{a}{2}\right)(\hat{x} + \hat{y} + \hat{z})} \right] \\ &= f \left[ 1 + e^{-i\vec{x}\cdot\left(\frac{a}{2}\right)(\hat{x} + \hat{y} + \hat{z})} \right] \\ &= f \left[ 1 + e^{-i\pi(h+k+l)} \right] \\ &= f \left[ 1 + (-1)^{h+k+l} \right] \end{aligned} \quad (15)$$

Thus, the structural constant for the surface  $(hkl)$  is indicated as follows:

$$F_{hkl} = \begin{cases} 2f & , \quad h+k+l \text{ 益?} \\ 0 & , \quad h+k+l \text{ 管?} \end{cases} \quad (16)$$

It means, in order to create the reflection in the diffraction experiment for a BCC crystal, the sum of the indices connected to the surface should be even. If the sum of the Miller indices is odd, The intensity of the beam will be scattered and will reach zero. Besides, the interference would be destructive and the zero status in the intensity happens alternatively. The most intensity of diffraction occurs in BCC solid on surface (110).

### 3. Collecting data and consequences

In this part, we attempt to put the density distribution function relevant to BCC crystal into the theory and then calculate *Helmholtz* free energy. But prior to this, it is rational that some of the theoretical and practical results of this method should be explained and at least we must know that what kind of results we are looking for in the end. The formulation of the Interface between a solid and liquid has been always controversial. From the experimental perspective, contact of two surfaces is related to two condensed matters. It is obvious that acquiring the contact information throughout using practical methods directly, appears to be a little difficult. Therefore, in this situation indirect parameters are measured. As an illustration, these two states of condensed matters adjacent together, make another kind of material as a result of the interactions and their influence on each other. But from the theoretical view, contact mechanism is considered to be the same for both materials. From this point, interaction between solid and liquid is divided into two categories: the first one is the solid in a liquid of the same material, in this state, the structural changes should be surveyed. The second one is related to the liquid and solid which are not the same, in this case, thermodynamic and chemical behavioral differences are studied.

Atomic modeling provides specific condition to simulate both phases and it also aids us to find a nearly direct approach so that the atomic interactions with ease. *Kerbekht* model and *Lennard-Jose* model can be good samples of the mentioned approach.

In the first state, the similar solid and liquid, experimental and empirical results indicate that the done interaction occurs in the first layers of the solid in the vicinity of the liquid. For example, In *Huisman* investigation, this experiment has been done with liquid Gallium and the surface of the diamond - (111)- it is noticeable that the phase of interaction decreases dramatically when it gets away from the surface. In the usage of surface (100), it is also witnessed. This result can be harvested that the fluid in the vicinity of

the surface behaves like a semi-solid or quasi-solid. But we have not had appropriate details regarding the impacts of solid on the liquid phase, yet.

This method, through the modeling of interaction in the forms of interaction connected to the tough sphere with a hard surface, the tough sphere with the elastic surface and finally the hard sphere with a liquid surface has been done.

The approximation of the weighted density function has been used In the first two cases while the modified theory of the weighted density function has been considered in the third issue. The main notion of computing in all the mentioned methods is generated by the *Basiyoun Partour* extension and the major potential function such as *Bolutzman* function -  $\exp(-\beta\phi_w)$ .

In this equation,  $\phi_w(\mathbf{z})$  is termed with the interacted potential between tough sphere and the surface.

By using this method, the profile of fluid density in the vicinity of solid surface is obtained which indicates that the liquid phase has been made in layer forms. By increasing the distance of  $z$  from the surface, the density of the corresponding layers has been declined. These consequences present that lamination the liquid in adjacent the solid strongly depends on the attraction and repulsion of both surfaces. It exactly means the same thing had been presented in *Vanderwaals* theory. There exists a significant point, the main and crystal structure has been considered the solid, that is why the results still are not very accurate. Next, the interaction between BCC solid and its molten phase were examined. But the same potential function for interaction had been still taken which was a function of the direct distant among the surfaces. Since this was one-dimensional prototype, so for different surfaces and various directions, it obtains diverse values. In accordance with the final interaction is a function of individual interactions among two phases atoms. In addition, first, the average two-dimensional of  $\phi_w$  was measured on all surfaces. Subsequently, a spectacular result regarding interaction with the surface was accomplished. Certainly, Boltzmann function was used in this computation.

In figure 2, the mentioned potential for surfaces 111 and 100 related to BCC solid have been indicated. The density profile related to the surfaces has been presented (Figure 2). As illustrated in the diagram, you could recognize how the density declines when the distance rises. Furthermore, it is clear that both corresponding graphs experienced volatile changes. Besides, the damping of fluctuations is highly similar together and finally the amount of density reaches approximately a quarter of the initial value. The

similarity of the profile relevant to both surfaces shows that we have taken the right method. In addition, there exists an appropriate relation amongst the consequence of calculations.

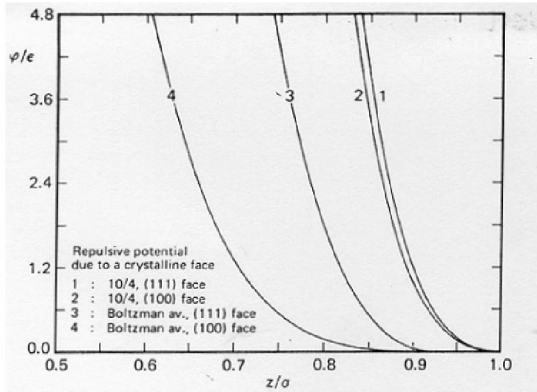


Figure 2. Interaction potential due to the crystal surface in term of the surface 111 and 100

As we mentioned before, the density function of solid-fluid system in Fourier analysis and based on the wave vector -  $K_n$  - in the reverse space of the solid network is introduced as follows:

$$\rho(v) = \rho_0(1+n) + \rho_0 \sum_n \mu_n \exp(ikn.r) \quad (17)$$

In the above formula,  $\{x_n\}$  is the sum of the reverse vectors in solid network,  $n$  is the coefficient of density variation during solidification and  $\mu_n$  is Fourier coefficients.

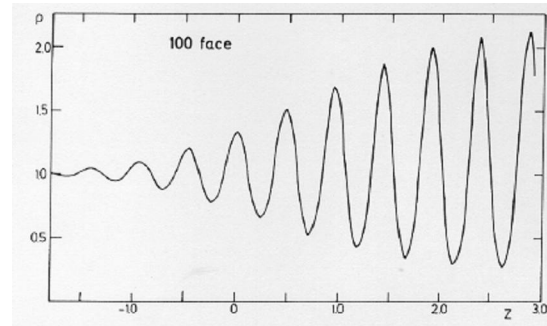
In fact, all vectors of reverse network in the mentioned series will not be existed. So, those vectors which are the closest neighbors will be considered. It happens because the role of the farther vectors in density is less effective.

Hence the application of the theory will be restricted to the crystals which have numerous close vectors. For instant, this issue is considered in solid BCC which has 12 first-neighbor and 12 vectors of the reverse network. Indeed, this notion causes this series be convergent readily. As an illustration, in solid SC which has only 6 first neighbor, six vectors are considered however appropriate results are not obtained.

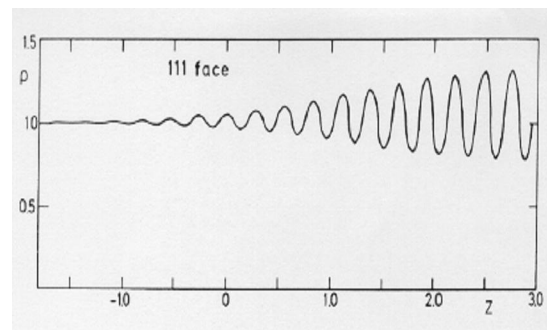
For FCC solid, two Brillouin zones should be considered. Of course it had not been done previously and the used approximations had not been actual. Our investigation contains Geometric corrections (reverse space vectors) and interaction energy between the solid and fluid.

The first result of the corrections is related to obtain various consequences for different surfaces. For instant, for surfaces (100) and (111) in BCC solid

-as seen in figure 3- it could be concluded that the structure of the fluid adjacent to the solid possesses a density of a distinct liquid-like. But the solid will have the constant structure. This interaction will have a range of  $20-16\text{\AA}$  and it includes nearly 5-10 layers. Comparing profiles of surfaces (111) and (100) in BCC solid, it is concluded that it would be alternative significantly and the approximation of interaction between fluid phase and other various layers is also obtained. If the density of fluid is  $\rho(v)$  and the density of fluid-like is  $\rho(\theta)$ , just under this circumstance:  $\Delta\rho \ll 1 \cdot \Delta\rho = \rho(v) - \rho(\theta)$ , jump density could be ignored near the iced point of fluid. Furthermore, if  $\Delta\rho$  changes slightly, it could be concluded that the vibrations of the density declines by increasing the distance and it is eliminated with the distance  $z$  from the surface. It means that the existence of the solid contributes to the process of internal changes in fluids to be done fast.



a



b

Figure 3. Density profile in term of distance. a: surface (100), b: surface (111)

Since we are not going to check the consequences, we complete this issue by discussing the graph related to the interaction of solid BCC and liquid. Based on figure 4, we could recognize what processes happen at the zero point- the boundary of solid substance.

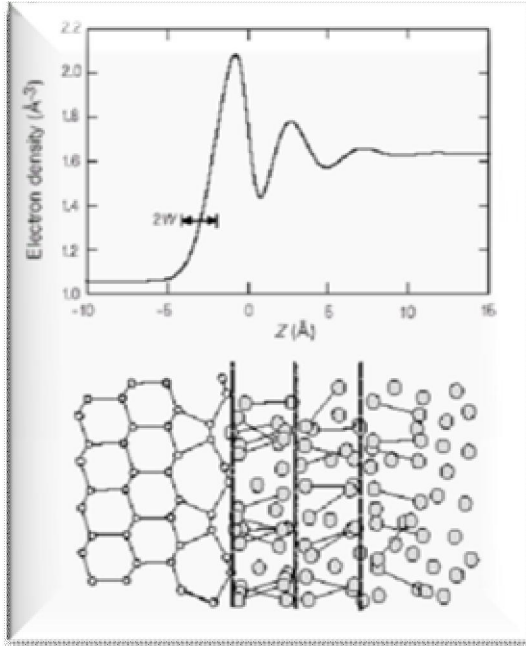


Figure 4. The curve of electron density in terms of distance

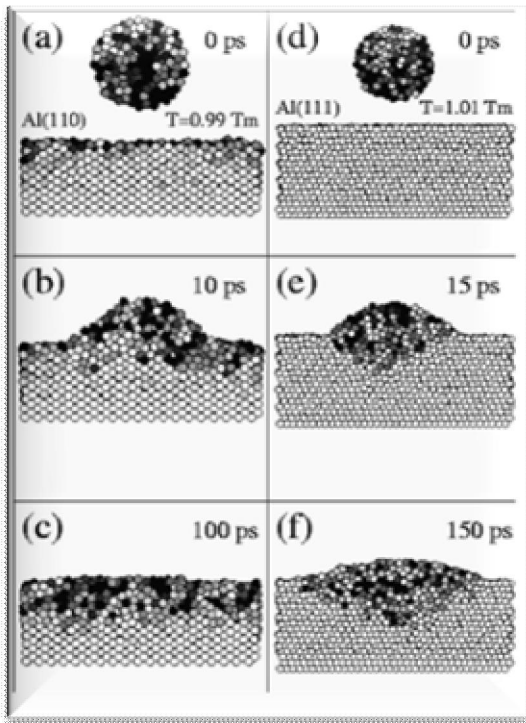


Figure 5. Schematic image of interaction in Aluminum close to its melting point.

In this section, we are going to illustrate a suitable instant related to the interaction between faces 111 and 110, then the differences are checked. For face 110 at 99 degrees Celsius ( it is exactly 1 degree below the melting point), we poured one drop

of Aluminum on the surfaces 110 and 111. The drop contains 861 solid particles and 16 layers. It is witnessed that the melting point for the final surface is much more smooth in the below interaction. At the higher temperature of the melting point, because of phase changes and also in accordance with the time which is required more to complete the interaction, the attained surface is rougher that the previous state. This matter will be discussed in the applications section.

Density profile  $\rho(z)$  as the average density of particles along the length  $\Delta z$  in parallel to the solid surface and  $z$  is defined as the length of the spot. The sub-surface is divided into two physical layers. The function of density profile is:

$$\rho(z) = \frac{\langle N_z \rangle}{L_x L_y L_z} \tag{18}$$

Where  $L_x L_y$  is the dimension of the cell in directions  $x$  and  $y$ , so that it will be perpendicular on direction  $z$  and  $L_z$  is the length of the middle part.  $\langle N_z \rangle$  is the number of particles which are located between  $z - \frac{\Delta z}{2}$  and  $z + \frac{\Delta z}{2}$  in the period  $t$ , the average value will be the average time. Potential function of each particle is introduced as follows:

$$U_p = \sum_{i \in L} u_i / N(L) \tag{19}$$

Where  $N(L)$  presents the quantity of atoms belonging to the layer,  $u_i$  is the amount of interaction energy relevant to the particle  $i$  and finally,  $L$  is the sum of the all particles in the layer. So, the temperature of each layer could be calculated from the equation:

$$T = \frac{2E_x^L}{3N(L)_{x_B}} = \frac{1}{3N(L)_{x_B}} \sum_{i \in L} \left| \frac{u_i}{V_i} \right|^2 \tag{20}$$

Where  $E_x^L$  is the kinetic energy of layer  $L$  and  $V_i$  is the velocity of the particle  $i$ . In the calculations, units are taken into account that the mass of the particle is assumed one. Thus,  $V_i$  would be the same momentum. Now, parameter  $S(x)$  is defined as follows:

$$s(x) = \sum_{i,j \in L} e^{i x \cdot (v_i - v_j)} / |2/N(L)|^2 \tag{21}$$

In the above equation,  $x$  is the vector of the reverse network. We can now calculate the radial

distribution function of two-dimensional with ease. Certainly, we know that the radial distribution function of three-dimensional is the below form:

$$\rho g(v) = \langle \sum_{ij \in \Omega} \delta(r - v_{ij}) / v \left( \frac{1}{v_i}, v, \Delta r \right) \rangle / N(L)$$

$v_i$  is the atom location  $i$ ,  $v_j = \left| \frac{1}{v_i} - v_j \right|$  is its displacement,  $p$  is the volumetric density and  $v \left( \frac{1}{v_i}, v, \Delta r \right)$  is the spherical coplanarity with the center  $\bar{r}$  and diameter  $v$  and thickness  $\Delta r$  and  $\langle \rangle$  is the average time on the concurrent routes and  $\delta$  is the same Kronecker delta.

If you assume that  $h_n$  is the number of atoms which are in the form of  $(i, j)$  in  $n$  of this layer, it means that they are the ones which are true under this circumstance  $(n - 1)\Delta v < v_j < n\Delta v$ . The mentioned function at the point  $\bar{r}_n = (n - 1/2)\Delta v$  will be in the below form

$$g(r_n) = \frac{V(L)h_n}{2\pi N(L)^2 r_n^2 \Delta v} \quad (23)$$

By the replacement  $A(L)$  instead of  $V(L)$ , this below equation is obtained:

$$g(r_n) = \frac{A(L)h_n}{\pi N(L)^2 r_n^2 \Delta v} \quad (24)$$

Where  $A(L)$  is the top surface of  $L$ . Normalization coefficient has been chosen so:

$$g(r \rightarrow \infty) = 1 \quad (25)$$

In fact, everything which is located at the range of  $r$ , it ends to half of the shortest length of the layer. In accordance with Fourier analysis:

$$S(x) = 1 + \rho \int g(v) \exp(-ix \cdot r) dv \quad (26)$$

In an isotropic system, we have:

$$S(x) = 1 + 4\pi \rho \int \frac{\sin xr}{xr} g(v) v^2 dv \quad (27)$$

Now, the results of the calculation concerning solid BCC are described briefly below:

The profile of density for  $(100)$  BCC<sup>-A</sup> at three alternative temperature has been shown in figure 6 and the diagrams relevant to  $(110)$  BCC<sup>-A</sup> are plotted

in figure 7. Where, the rate of changes is constant and the density of the average numbers of two layers to the density of the liquid is transitioning. Anyway, it is remarkable that in BCC (100), the first peak of the liquid happens approximately  $0.615A^2$  from the surface continuously. This occurrence is indicated more accurately in figure 8. The first two peaks are related to the solid. In addition, another high peak is witnessed so close to them.

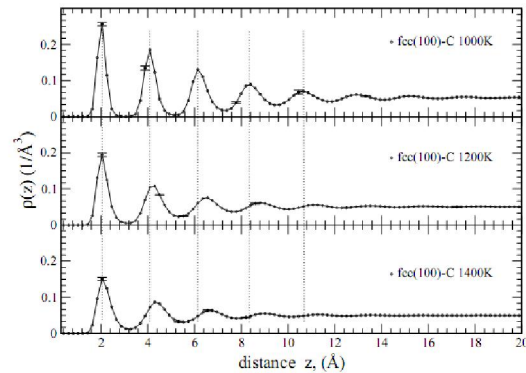


Figure 6. The diagram of density function for FCC solid based on distance at various temperatures.

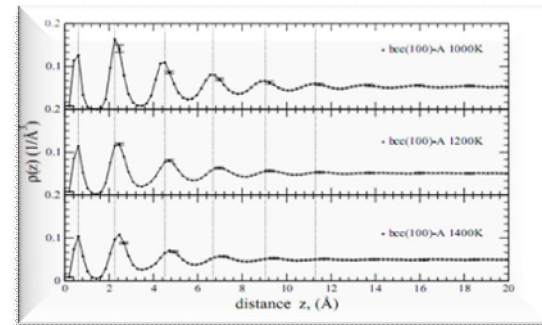


Figure 7. The diagram of density function for surfaces A of BCC solid based on distance at various temperatures.

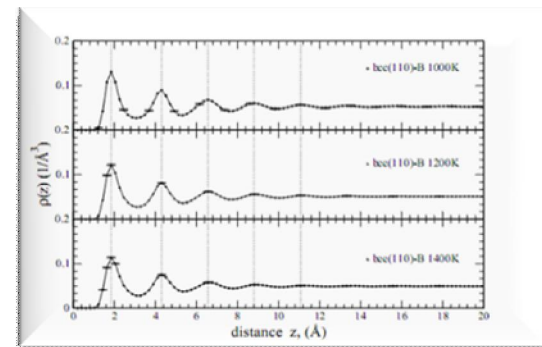


Figure 8. The diagram of density function for surfaces B of BCC solid based on distance at various temperatures.

**4. Review and explanation**

We have already explained the modified theory of the weighted density function and the attributes of solid BCC. On the other hand, we have investigated the interaction of solid and liquid states. By this way, we have shown how thermodynamic functions such as dependent energy and free energy change. Through this method, the density function has been attained upon the phase space. In addition, specific explanations regarding the mechanism of the interaction in a variety of solid states have been evaluated. Now, considering all the afore-mentioned details, it is time to conclude whatever we obtained and then we express the characteristics of the main model. Besides, we ought to present how our findings will convert into practical use. As far as we remember, the interaction occurs in all transitions of solid and liquid phase. For example, when the color layer reaches the metal face, it covers the surface Or when the insulating layer of the fluid should cover the holes on a surface. Even it is used in the coating layer in vacuum conditions and in computing the amount of adhesion to the substrate, whether the face is metal or non-metal. First of all, the simple and functional model is extracted from complicated equations and then we use it for various applications. It is emphasized again that for the non-uniform classical fluid, the same approximation related to tough spherical molecules are assumed and typical correlation functions are used for the solid. Under this condition, even in the simplest case, we will be forced to do the calculation relevant to non-metallic sequences. Our computations have been done analytically with considering specific approximation. So, accurate and statistical calculations are postponed until another time. The approximation for the modified weighted function would be in the following form:

$$\int_{\mathbb{R}^3}^{MWDA} P / N = f \cdot (p) \tag{28}$$

$$P = \frac{1}{N} \int \mathbb{R}^3 P(r) \int \mathbb{R}^3 p(r) w(r, r', p) \tag{29}$$

Where:

$$\int \mathbb{R}^3 w(r, r', p) = 1$$

Therefore, the density function would be in the below equation:

$$P(r) = \frac{1}{N} \int \mathbb{R}^3 p(r) \int \mathbb{R}^3 p(r) \tag{30}$$

At the first step, the first Brillouin zone for the solid is considered. Apparently, in the equation,  $N=8$

and  $r$  is the same basic vectors in solid BCC network based on the below figure:

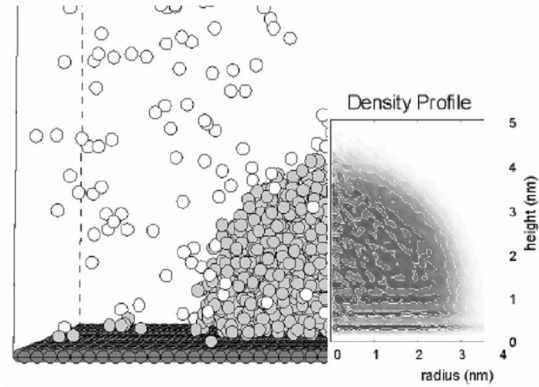


Figure 9. The schematic diagram the first stage liquid-solid BCC interaction

In this section, we consider the contact process of a liquid or solid substance with ease based on the approximations and findings in the previous chapters. As we know, realizing the sequence has numerous impacts on the phase changes on the contact cross-sections, the adhesion and superficial adhesion of fluid phase with solid and other vital parameters. In a similar process based on molecular approaches, it is possible to use these achievements so as to investigate the amount of liquid formed on the solid surface at the saturated vapors. In the same way, the difference between mechanical and thermodynamic methods and macroscopic ones is just in the determination of balance line related to three different phases of the substance. Through this method, the rate of heat transfer on contact surface could be obtained. But based on whatever we achieved, molecular dynamics methods are the best one to reach this goal and macroscopic simulation ways have numerous limits in calculations. Nowadays, this process in some nanotechnological usages (such as getting wet metallic catalysts in numerous fuel cells) for this purpose, using the WDMA or molecular dynamics approaches are highly recommended.

Furthermore, by this way, it is possible to make a rational comparison between nanoscale systems and macroscopic ones. Through this approach, the possibility for producing them is provided. In order to simplify the process, Lennard – Jones potential for the model of liquid phase is used and a BCC solid is also considered for simulating of solid phase.

Some particular cases would be surveyed through this investigation. For instant, we will carry out how to spread on the solid surface, the final shape of diffusion and spreading liquid bubble on the solid face or even thermal resistance. Obviously, the close layers to the solid surface located on the first



Merbeliubin are considered. So as to calculate the values, Young equations are used. In this stage, the corresponding base metal is a kind of Platinum having BCC structure. Just as we know, the corresponding potential would be as follows:

$$Q(r) = 44 \left\{ \left( \frac{r}{r_0} \right)^{12} - \left( \frac{r}{r_0} \right)^6 \right\} \quad (31)$$

Where:  $m=6/63 \times 10^{-26}$  ng,  $\epsilon=1/67 \times 10^{-21}$  J and  $\sigma = \frac{3}{40} A^D$ .

It is Also possible to determine the existing potential on the biphasic surface in this same function with the energy variable NT till  $\epsilon$ . Besides, the interaction of  $\sigma ENT$  is obtained based on the face. The primary variables related to the harmonic potential of the solid surface layer, mass, spring constant coefficient and the factor line of the occupied network for Platinum are determined. A view of a contact of the liquid with the two-dimensional density profile and solid surface is plotted in figure 9.

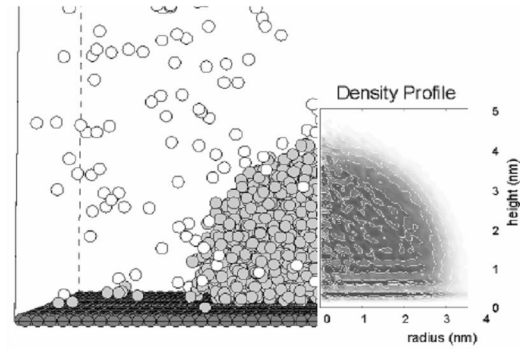


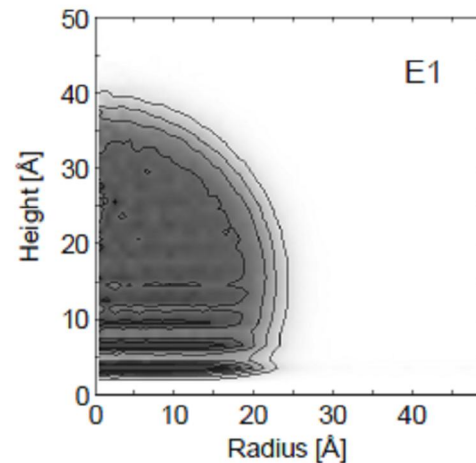
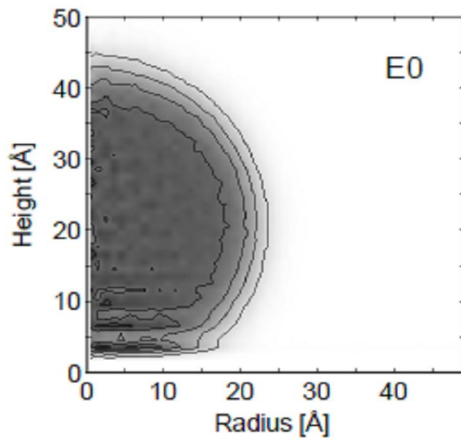
Figure 10. A view of the contact the liquid with the solid surface and its two-dimensional density profile in nanoscale.

The impact of potential on the interaction of the hitting liquid surface with solid has been indicated in figure 10. In the same way, potentials of the interaction NT till  $\epsilon$  at the temperature of 100 degrees for six states have been presented on table 1.

Table 1. potential values of interaction  $\epsilon ITN$  and contact angle at 100 degrees Celsius.

	surf $\epsilon$	$\epsilon INT \{10^{21}j\}$	$\theta [deg]$
$E_0$	0/73	0/228	
$E_1$	1/29	0/404	135
$E_2$	1/86	0/581	110
$E_3$	2/43	0/758	79
$E_4$	2/99	0/935	49
$E_5$	3/56	1/112	

It is witnessed that by increasing the amount of the potential interaction on surfaces, the adhesion of the liquid to solid surface rises. Furthermore, by possessing a strong potential interaction, separating the first surface of liquid, after hitting, is too difficult.



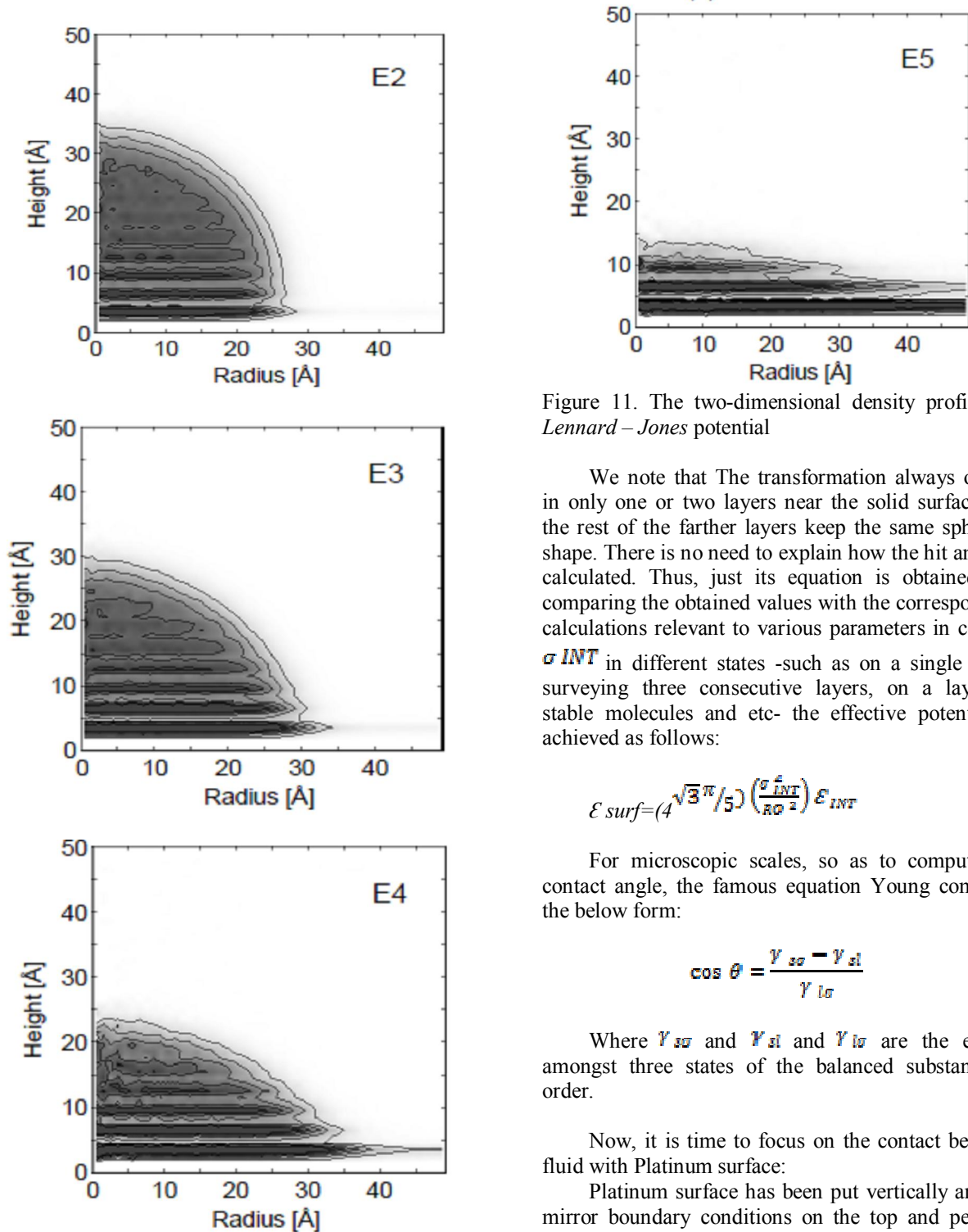


Figure 11. The two-dimensional density profile for Lennard – Jones potential

We note that The transformation always occurs in only one or two layers near the solid surface and the rest of the farther layers keep the same spherical shape. There is no need to explain how the hit angle is calculated. Thus, just its equation is obtained. By comparing the obtained values with the corresponding calculations relevant to various parameters in contact  $\sigma_{INT}$  in different states -such as on a single layer, surveying three consecutive layers, on a layer or stable molecules and etc- the effective potential is achieved as follows:

$$\epsilon_{surf} = (4\sqrt{3}^{\pi}/5) \left( \frac{\sigma_{INT}^6}{R0^2} \right) \epsilon_{INT} \quad (32)$$

For microscopic scales, so as to compute the contact angle, the famous equation Young comes in the below form:

$$\cos \theta = \frac{\gamma_{ss} - \gamma_{sl}}{\gamma_{ls}} \quad (33)$$

Where  $\gamma_{ss}$  and  $\gamma_{sl}$  and  $\gamma_{ls}$  are the energy amongst three states of the balanced substance in order.

Now, it is time to focus on the contact between fluid with Platinum surface:

Platinum surface has been put vertically and the mirror boundary conditions on the top and periodic boundary circumstances are existed in all four directions. For Platinum surface, three layers of Identical molecules are considered. In various potential function, there is the first cross-section which each round of them is extracted from developing of spherical Henkel functions in biphasic distribution of contact surface.

Certainly, there is another potential function

which we do not use and just introduce it.

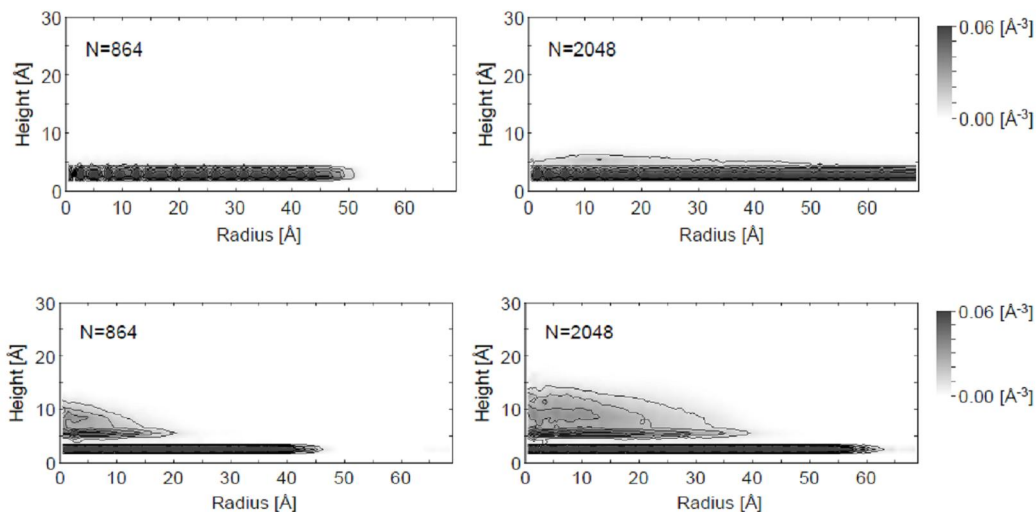


Figure 12. The two-dimensional profile of density in contact with liquid to surface BCC 111  
 A: considering our potential function  
 B: with other potential functions

The distribution of two-dimensional density of the liquid on surface BCC (111) is presented in figure 11. In the tube model, the fluid covers the surface so that only one layer is left. This limit does not exist in

the second model. The mechanism of the contact between liquid phase and solid was examined in two mentioned models in figure 12.

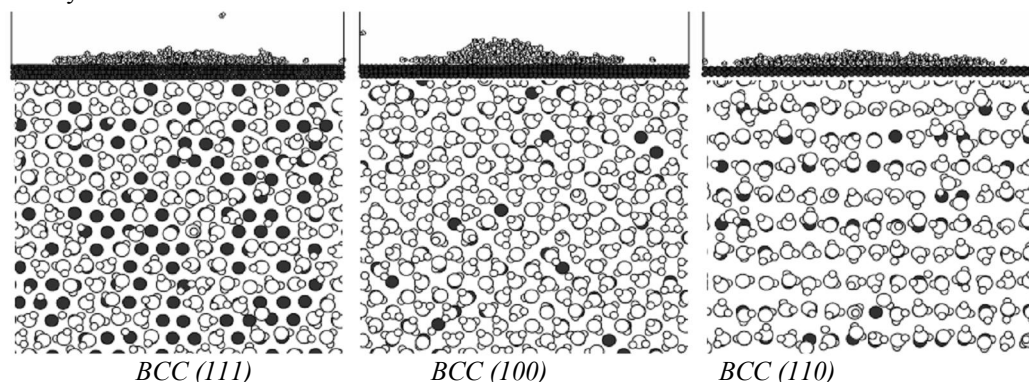


Figure 13. The mechanism of the contact between the liquid and the solid surface in the first layer of the first model

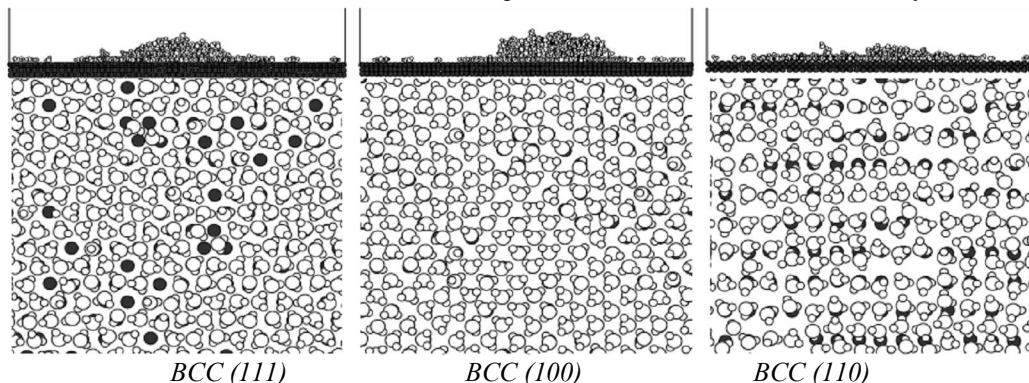


Figure 14. The mechanism of the contact between the liquid and the solid surface in the first layer of the second model

We understand that the amount of the density is large, medium and tiny for surfaces 111, 100 and 110, respectively. For surfaces 100 and 110, fluid molecules cover all the surface entirely. But the superficial density of the atom in surface 111 is enormous. Hence it could not cover it completely.

So the most efficiency in the process will be existed on surfaces 110 and 100. This approach is used in resin and color industries directly.

## 5. Results and discussions

In this part, the usages of these outcomes are surveyed in color industry. As we obtained, one drop of a fluid stuck to the solid surface through a specific mechanism which is different due to the type of solid. Results present that the potential of the solid surface is more and the viscosity of the fluid increases, surface adhesion will be more. In the same way, based on the structure of a BCC solid, it is concluded that the surfaces (110) operate more efficiently than surfaces (100). By carrying out the experiment at a variety of temperatures and different substances, it could be noted that the temperature of the interaction environment impacts on the behavior of two surfaces.

Eventually, the fusion and ingrowing values rises. Another vital point applied in industries is related to the temperature of the chamber which the solid is kept in should be nearly 20 degrees less than the temperature of the reaction flask after the interaction.

In practice, use of these outcomes requires simulating the corresponding process in experimental circumstances. It means that a model for the contact of the liquid -which might be epoxy resins or oil paints- should be designed with the BCC surface, moreover, its attributes are tested.

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