Numerical study of the effect of the structural disorder on the electronic properties in disordered solids.

A. Houari[1], M. Ould Mohamed[2], T.Ouahrani, M. Mebrouki and A. F. Dib

Laboratoire de Physique Théorique - Département de Physique- Faculté des sciences-

Université Abou Bakr Belkaïd- B.P. 119 Bel Horizon 13000 Tlemcen Algérie.

During the last few years, it became clear that the characterization of the nature of electron states in disordered systems is one of the fundamental topics in condensed matter physics. Along these lines, our present work consists of the study of the effect of the structural disorder on a wide range of electronic properties (density of electron states, participation ratio of electron states and distribution of energy levels). For this, we generate the structural disorder according to three different models: a model named "*Shaken lattice'',* a model simulated by *molecular dynamics* and the model of the *random triangles.* Concerning the Hamiltonian model, we use a Tight-Binding model with explicit S-type orbitals for the first two structures and a *clean* Tight-Binding model for the model of the random triangles. Our results show that electron states are localized or delocalized depending on the type of the structural disorder used to generate a particular topologically disordered system.

Key-words: st*ructural disorder, random matrices, electronic localization, Shaken lattice, molecular dynamics, random triangles.*

I INTRODUCTION:

The characterization of electron wave functions in disordered systems has been one of the main interests of condensed matter physicists. The focus has been particularly for some period of time on the nature of the structure of the electron wavefunctions and their energy level statistics at the metal-insulator transition. In these works, most of numerical approaches mainly considered susbtitutional disorder paying little attention to topologically disordered systems because the generation of the latter is not straightforward. Only recently, topologically disordered systems such as amorphous solids, liquids, polymers and quasi-crystals are a subject of intensive research projects. These systems require condensed matter physicists to develop realistic models to simulate them. Among existing models, we mention here as an example random Voronoi tesselations [1] which are largely used in condensed matter physics. Along these lines, we particularly focus here on the effect of varying the type of the topological disorder on the nature of the electron wavefunctions. For this, we consider three different models to generate topologically disordered structures. The first model is the *Shaken lattice* model [2] which generates site positions of the disordered structure in a random way starting from a periodic lattice. The second model is simulated by *a* molecular dynamics algorithm [3]. The last model simulates the random structure by generating random bonds between the sites of a 2-d periodic lattice (the *random triangles* model [4]). To the best of our knowledge, there is no such an investigation in the literature examining the effect of varying the type of the topological disorder on the nature of electron wavefunctions.

II CONSTRUCTION OF THE STRUCTURAL MODELS:

Our starting model is a substitutionally disordered binary alloy A_cB_{1-c}. By the latter, we simply mean a regular 2-d square lattice of lattice constant *a* where a fraction c of the sites are occupied by atoms A with the strength of the potential γ_A and the rest are occupied by atoms B with strength γ_B. We further assume that the site occupancies are uncorrelated so that the probability that any site is occupied by the A-species is c_A=c, the concentration of the A-species, and the probability that any site is occupied by the B-species is c_B=1-c, the concentration of the B-species. The probability distribution for the strengths of the potential γ_i is thus given by:

$$p(\gamma_i) = c\delta(\gamma_i - \gamma_A) + (1-c)(\gamma_i - \gamma_B) \quad (1)$$

Our ''Shaken lattice'' (SL) model [2] which simulates a topologically disordered structure is constructed from the regular structure of substitutional disordered binary alloy by considering a single atomic species and moving each atom, considered as a hard circle of radius *r*, by random displacements from its lattice site (See figure 1). In terms of equations, we write:

$$\begin{cases} X_{dis} = X_{ord} \pm \delta x \\ Y_{dis} = Y_{ord} \pm \delta y \end{cases} \qquad (2)$$

where X_{ord} and Y_{ord} represent coordinates of sites in the periodic lattice.

X_{dis} and Y_{dis} are coordinates of sites in the disordered structure.

δx and δy represent random displacements having uniform distribution in the interval $\left[-\frac{\theta}{2}, \frac{\theta}{2}\right]$ where θ represents the degree of topological disorder with $-a+2r < \frac{\theta}{2} < a-2r$ (in our case a=3., r =1.)

For the simulation of the topological disorder by the molecular dynamics (MD), we refer to Ref. [3] where the simulation algorithm is described in detail. Finally, for the random triangles model, we start from a 2-d periodic system

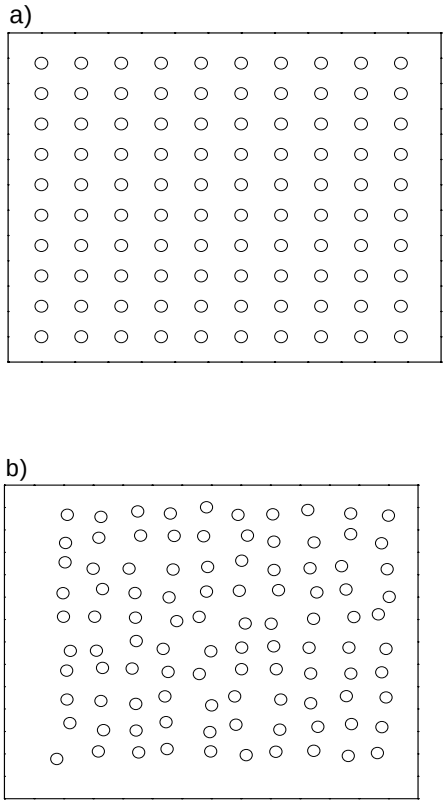

FIG 1: Graphical representation of sites in two-dimensional system simulated by *Shaken lattice* model with: a) θ=0.00, b) θ=0.60

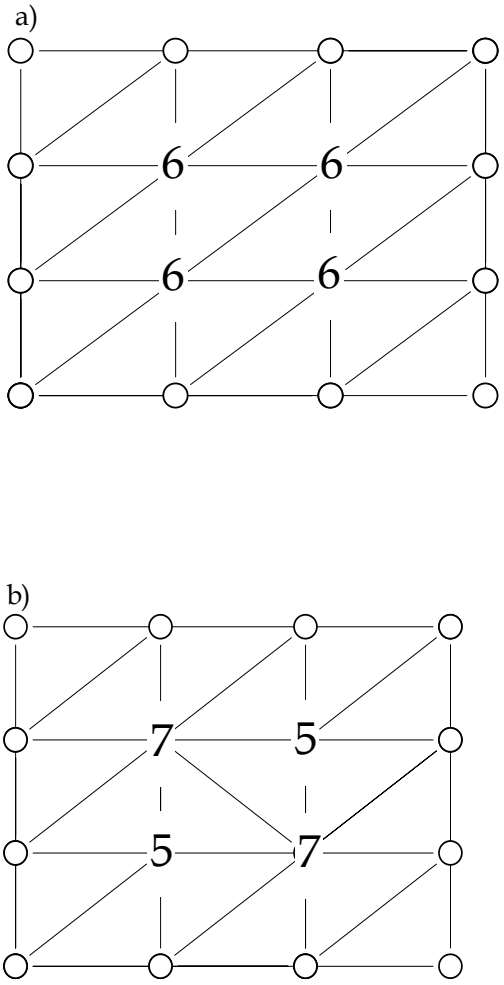

FIG. 2 : a) Ordered triangles. b) Random triangles: numbers indicate the numbers of nearest neighbour sites for each site

where each site has six nearest neighbors as shown in figure 2.a, the structural disorder is introduced by varying randomly the number of the nearest neighbor sites of each lattice site. This is made by random flips of diagonal bonds (see figure 2.b).

III HAMILTONIAN MODEL:

In this paper, we use a one-electron Hamiltonian model which is defined in real space for the first two disordered structures (the *Shaken lattice* and the amorphous alloy simulated by *molecular dynamics)* .This Hamiltonian model is given by:

$$H = \frac{p^2}{2m} + V(\vec{r}) \qquad (3)$$

where $V(\vec{r})$ is the potential of the system obtained as superposition of atomic-like potentials U_i centered at each site of the system:

$$V(\vec{r}) = \sum_i U_i = \sum_i U(\vec{r} - \vec{R}_i) \qquad (4)$$

We choose here a simple δ potential which simulates a short-ranged interaction characterized by single parameter. This choice goes to the limiting version of the Hulthèn potential when the radius of the region within which the force acts tends to zero. To accomplish this limit, we have to send both parameters b and q of the Hulthén potential to infinity in such way that the ratio $\frac{b}{q^2} \to \frac{1}{2}$. This limit is convenient because it determines U by only the parameter γ, given by $b = \gamma q + \frac{q^2}{2}$

$$U(r) = -b\frac{\exp(-qr)}{1-\exp(-qr)} \qquad (5)$$

The potential U has only one bound state at energy E given in atomic units by E = $-\gamma^2/2$ with the normalized wave function [5] :

$$\phi(\vec{r}) = \left[\frac{\gamma}{2\pi}\right]^{\frac{1}{2}} \frac{\exp(-\gamma r)}{r} \qquad (6)$$

By using the set of the atomic orbitals $\{\phi(\vec{r} - \vec{R}_i)\}$ for the Hamiltonian in the tight-binding model, the Hamiltonian matrix elements are given by:

$$H_{ij} = \langle \phi_i | H | \phi_j \rangle \qquad (7)$$

After some manipulations [2], the Hamiltonian matrix elements are:

$$H_{ij} = \varepsilon_j S_{ij} + \langle \phi_i | U_i | \phi_j \rangle \qquad (8)$$

$\varepsilon_j = \frac{-\gamma_j^2}{2}$ represents the site energy which is the eigenvalue of the *Schrödinger* equation for an isolated atom in the state $|\phi(\vec{r} - \vec{R}_j)\rangle$

S_{ij} are the matrix elements of the overlap matrix given by:

$$S_{ij} = \int \phi^*(\vec{r} - \vec{R}_i)\phi(\vec{r} - \vec{R}_j)d^3\vec{r} \qquad (9)$$

$$S_{ij} = 2\frac{(\gamma_i\gamma_j)^{\frac{1}{2}}}{(\gamma_i^2 - \gamma_j^2)}\frac{\left(e^{-\gamma_i R} - e^{-\gamma_j R}\right)}{R} \qquad (10)$$

$$\langle \phi_i | U_i | \phi_j \rangle = -(\gamma_i\gamma_j)^{\frac{1}{2}}\frac{e^{-\gamma_j R}}{R} \qquad (11)$$

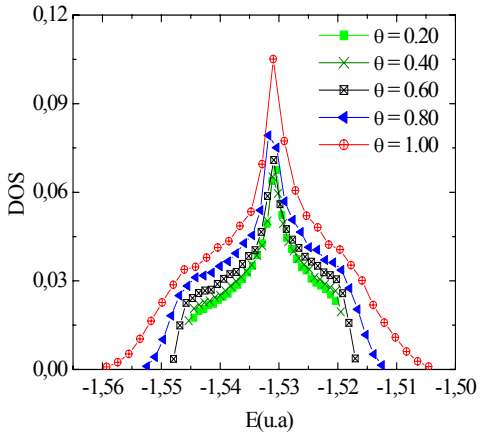

FIG. 3: Variation of the density of states with the disorder parameter θ for a topologically disordered system simulated by *Shaken lattice* model ($N = 45 \times 45$).

where $R = \left|\vec{R}_i - \vec{R}_j\right|$ is the distance between the site i and the site j. Finally, we obtain:

$$H_{ij} = \frac{\left(\gamma_i \gamma_j\right)^{\frac{1}{2}}}{\left(\gamma_i^2 - \gamma_j^2\right)} \frac{\left(\gamma_j^2 e^{-\gamma_i R} - \gamma_i^2 e^{-\gamma_j R}\right)}{R} \qquad (12)$$

The diagonal elements are given by:

$$\begin{cases} H_{ii} = \dfrac{-\gamma_i^2}{2} \\ S_{ii} = 1 \end{cases} \qquad (13)$$

and in the case where γ_i and γ_j are equal, the corresponding expressions are:

$$\begin{cases} H_{ij} = -\left[\dfrac{\gamma_i}{R} + \dfrac{\gamma_i^2}{2}\right] e^{-\gamma_i R} \\ S_{ij} = e^{-\gamma_i R} \end{cases} \qquad (14)$$

For the last structure, we use clean tight-binding model [4] (diagonal elements of the Hamiltonian matrix are equal to zero). This Hamiltonian takes the following form:

$$H = \sum_{i,j}^{N} t_{ij} \left|i\right\rangle\left\langle j\right| \qquad (15)$$

i and j label the site indices in the structure (two-dimensional in our case), *N* is the total number of the sites. t_{ij} is equal to 1 for nearest neighbors site and 0 otherwise.

.

IV- RESULTS AND DISCUSSION:

Before we start our numerical investigation of electronic properties, we first simulate the structural disorder in our models according the following parameters: for *Shaken lattice* model, $\gamma_a = \gamma_b = 1.75$ (γ_a and γ_b are the atomic potentials of atom A and atom B respectively) in 2-d system of size 45×45.

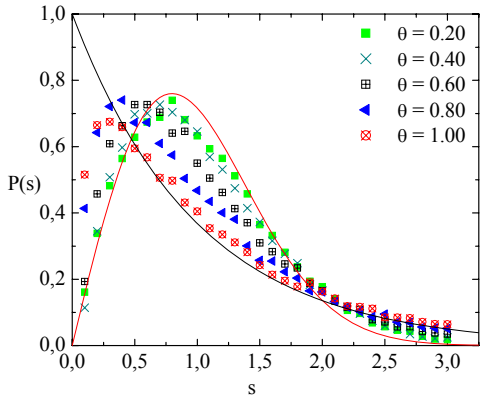

FIG. 4 : Variation of distributions of energy spacing *P(s)* with the value of θ for a topologically disordered system simulated by *Shaken lattice* model. (The full lines represent Wigner distribution (red) and Poisson distribution (black)).

For the disordered system which is generated by *molecular dynamics*, we take a sample of a binary alloy of size *1372 atoms* with the choice γ_a=1.85, γ_b=2.00. Finally, for the system of the random triangles, the degree of the structural disorder is given by the percentage *P* of the diagonal bonds having the same direction in space (the number of nearest neighbors of each site varies in a random way from one site to another one). In our case, we choose *P=50%* i.e. a maximum disorder and a size 45×45.

We start our study by looking at the variation of the density of electronic states (see figure 3) as a function of the value of the disorder parameter θ of the topologically disordered system (*Shaken lattice).* We note that as θ increases, the energy bandwidth increases. We represent in figure 5 the density of electronic states for the two other disordered structures. We notice that their curves have only one maximum due to the singularities rising from the analytical form of the density of states in the Fourier space (Van Hove singularities).

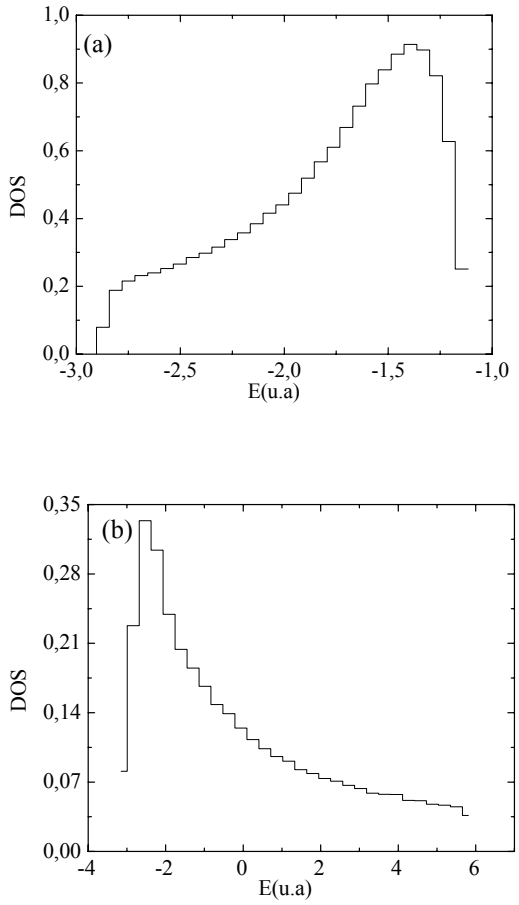

FIG. 5: density of states of a topologically disordered system simulated by: a) Molecular dynamics b) random triangles

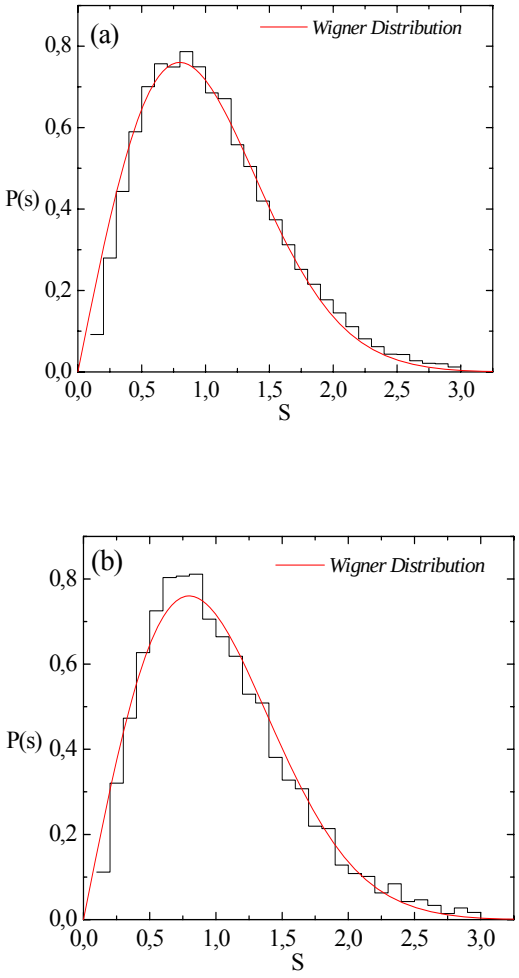

FIG. 6: distributions of energy spacing for a topologically disordered system simulated by: a) Molecular dynamics b) random triangles.

As we increase the value of θ, the curves of the distributions of energy levels spacing show a transition from a distribution characterizing extended states (metallic phase for θ=0.20) towards a distribution characterizing localized states (insulating phase for θ=1.00) (see figure 4). In figure 6, we represent the density of probability of energy levels spacing *P(s)* for the models (MD and RT) in terms of the normalized spacing. We note that *P(s)* follows the *Wigner* distribution characterizing the Gaussian Orthogonal Ensemble of symmetric random matrices [6]:

the probability of having two energy levels very close is very small compared to that having two energy levels spaced of a value equal to the mean spacing. This phenomenon is known in the literature by the energy level repulsion. Consequently, with our chosen parameters, our disordered SL and MD structures are in the metallic state.

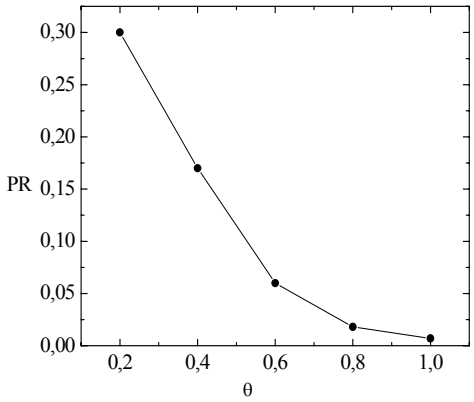

FIG. 7 : variation participation ratio *PR* with the degree of disorder θ for a topologically disordered system simulated by *Shaken lattice* model.

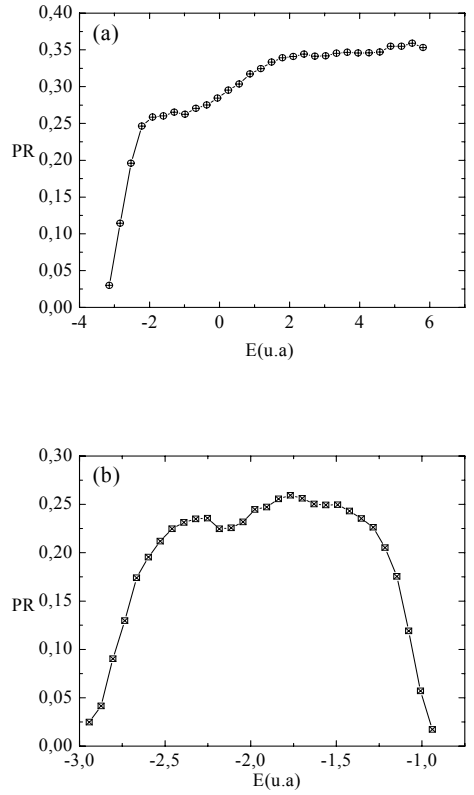

FIG. 8: variation participation ratio *PR* with the energy for a topologically disordered system simulated by: a) random triangles*;* b) molecular dynamics.

To examine the degree of the localization of the wavefunctions in our disordered systems, we use the participation ratio *PR* which gives the number of sites contributing to the spatial extent of the electronic state. To calculate PR we consider a wavefunction calculated from a tight-binding Hamiltonian model i.e. $\Psi_k = \sum_i a_{ik} \left| \phi_i \right\rangle$, PR is defined as [2] :

$$PR_k = \frac{1}{N} \frac{\left[\sum_{i=1}^{N} |a_{ik}|^2 \right]^2}{\sum_{i=1}^{N} |a_{ik}|^4} \qquad (16)$$

To test the influence of the disorder parameter θ on the degree of the localization of the electronic states in the SL model, we represent the participation ratio in terms of this parameter (figure 7). As expected, PR decreases with increasing θ values so that the θ parameter plays the role of the degree of disorder in the traditional Anderson localization model [7].

The amplitude of the electronic wave functions is shown in figure 9 with increasing θparameter.

We represent in the figure (8.a) the participation ratio as a function of the energy for the model of *the random triangles.* We note that the average value of *PR* fluctuates around the value 0.30 which is the signature of the delocalized regime. The amplitude of the wave functions is represented in figure 10 which confirms the metallic character where the electronic wave functions are spread over the entire system.

According to the average value of *PR* of the amorphous alloy (see figure 8.b), we state that the latter has a metallic character. Here, we must stress that that the construction of the amorphous alloy is based on a rigorous simulation algorithm with a physics controlled by parameters simulating a physical reality contrary to that of *Shaken lattice* being a simple artificial model.

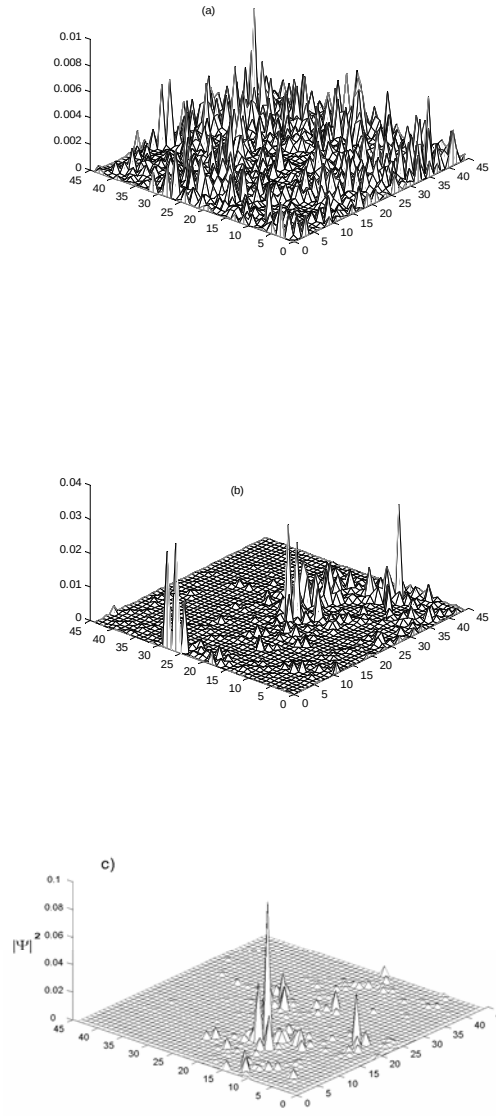

FIG. 9: graphical representation of the amplitude distribution $|\Psi|^2$ at the band centre for a topologically disordered system simulated by *Shaken lattice* model: a) delocalized state with θ=0.20. b) intermediate state with θ=0.60. c) localized state with θ=1.00

V- CONCLUSION

In this work, we showed that the topological disorder localizes electron states according to the used geometrical model for generating those disordered systems. We clearly showed that electron states are more localized in the system simulated by the *Shaken lattice* model than in the two other disordered

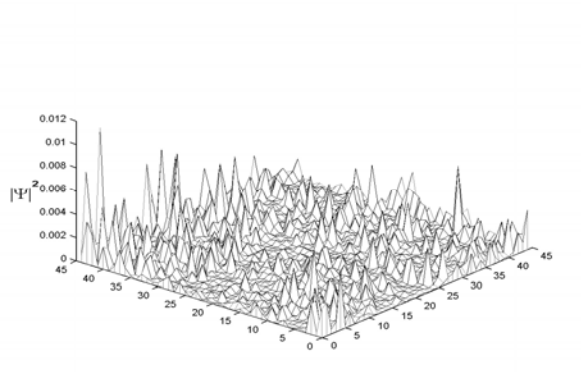

FIG. 10: graphical representation of the amplitude distribution $|\Psi|^2$ in the band centre for a topologically disordered system simulated by *random triangles* model.

structures where the metallic character was quite clear. Moreover the *Shaken lattice* model is a type of a disorder that localizes electron states slightly less than does the traditional energy-disorder Anderson model [7]. To complete the present study, we need to simulate the topological disorder using a more realistic inter-atomic potential in the molecular dynamics algorithm and using a much larger sample size to avoid any size-effect in our study. For this, we have to use more reliable numerical method such as Lanczos algorithm to solve the Schrödinger equation in the electronic structure problem. We intend to do that in the near future.

References

[1] N. H. Christ, R. Friedberg and T. D. Lee, Nucl. Phys. B **202,** 89 (1982)

[2] A. Houari, *Numerical Studies of Conductance Fluctuations in Disordered Metals*, Ph.D Thesis Mc Gill University, Canada (1990).

[3] A. Houari, M. Mebrouki, A. Dib, and F. Ould-Kaddour, *Physica B,* **29,** 378-393 (2000).

See also A. Houari, N. Benachour and A. Dib, *Moroccan Jour. of Cond. Matt*. **5**, 68 (2004)

[4] U. Grimm, R. A. Romer, and Schlieker, *Electronic States in Topologically Disordered Systems,* ArXiv: cond-mat/**9811360** v1 25 Nov (1998).

[5] A. A. Berezin, *Phys. Rev B*.**33**, 2122 (1986)**.**
[6] M. L. Mehta, *Random Matrices*, Academic Press, New York, 1991
[7] P. W. Anderson, *Absence of Diffusion in Certain Random Lattices*, *Phys. Rev*. **109**, 1492 (1958).