GROUPING MODEL IN FERMI SURFACE APPLIED TO QUASICRYSTALS

Nascimento, L.[1*]; Agostinho, L. C. L.[2]; Cavalcanti, F.B.[3]

[1*]Departamento de Física-*DF/CCEN-UFPB*
Cidade Universitária- Caixa Postal:5008-Cep:58059-900,João Pessoa-PB.
E-mail [1*]: **luciano.fisicaufpb@gmail.com**

[2]Departamento de Química-*DQ/CCT-UEPB*
Rua Juvêncio Arruda,s/n-Bodocongó-Cep:58109-790,Campina Grande-PB.
E-mail [2]:cristina.uepb@gmail.com

[3]Departamento de Hidráulica e Engenharia Civil-*DHEC/CCT-UFCG*
Av. Aprígio Veloso, 882-Bloco CM - 1°Andar - CEP 58.109-970,Campina Grande-PB.
E-mail [3:] bernardete.ufcg@gmail.com

ABSTRACT

Studies performed on energy levels in Fermi surface in groupings showed that crystals have plans periodically gathered. On the contrary, quasicrystals have their plans reunited non periodically. This paper shows the development of a mathematical model comprising not only the symmetries of AlMnPd alloys but also the physical stability of groupings versus AlCoNi geometry by considering Fermi energy in its surface. The model also discusses electron conductivity, quantum interfaces in quasicrystals, its physical formation and chemical properties. The model allows a better understanding of interactions between atoms in the quasicrystals formation, functioning of energy bonds and of gaps and pseudogaps in the electronic structures of quasicrystalline materials.

Key – words: Grouping; Symmetries; Fermi surface; Quasicrystals.

1. INTRODUCTION

Mathematical models for quasiperiodic structures are generally described by atomic groupings for modelling the structure of quasicrystals. Also, they contribute to understand the physical and chemical properties of quasicrystals. Groupings are tightly connected by covalent and metallic liaisons. This property was the basis to develop the Grouping Model for quantum formalism at the Fermi surface [1] presented in this paper.
Quasicrystals are atomic ordered structures that exhibit quasiperiodic translational order of a long range. These structures show forbidden crystallographic symmetries and are prepared by fast cooling techniques. Quasicrystals are good electric and thermal insulating materials. They exhibit unusual combinations of physical properties such as high hardness, low friction and good oxidation resistance. They also can be utilized as hydrogen source showing many advantages when compared to other materials[3]. Grouping Model shows examples of AlMnPd symmetries of 2/1 approximations in which a grouping of 9/12 spheres was derived with a 21, 21 Å diameter and was used to describe the structure in icosahedral phase [2].

These characteristics can be seen in the rotational spheres and are defined as a disorder in the icosahedral symmetry break of the AlMnPd quasicrystalline alloy as shown in Figure 1 [3].

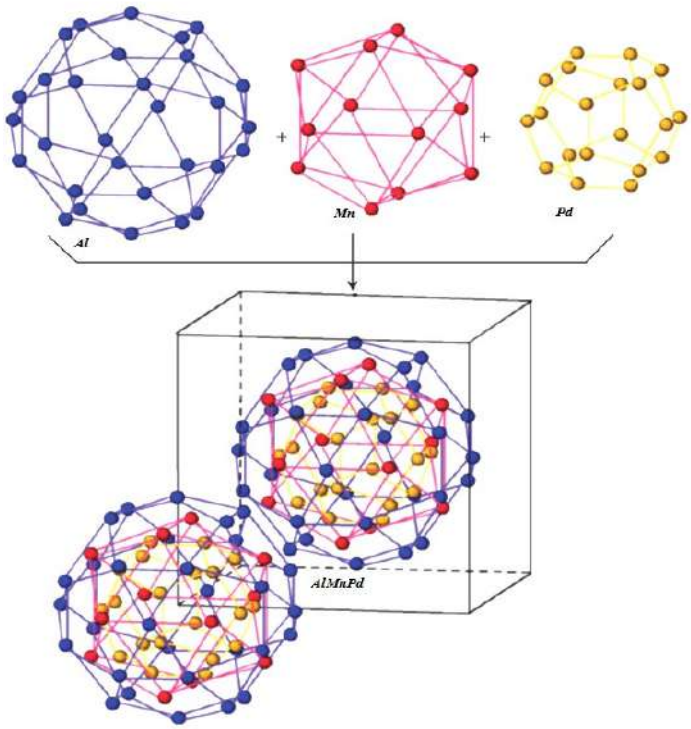

Figure 1. AlMnPd quasicrystalline alloy with grouping of icosahedral symmetry.

In the AlCoNi decagonal quasicrystal, the symmetry of grouping makes the structure of stability to present differentiated geometries. Between them and when the effects of Fermi energy are considered, an intrinsic disorder is observed [4]. Due to this performance, studies on quasicrystals groupings are becoming more intensive. More recently, the literature shows several studies on thermal, electric and magnetic properties of quasicrystals as, for instance, specific heat measurements studies.

2. THEORETICAL CONSIDERATIONS

At high temperatures, electrons are dispersed by vibrations of the quasicrystalline net. Consequently, a loss of moment of the resistivity is observed causing a structure disorder. At low temperatures, the dispersion between electron – electron is the dominant mechanism [5]. This behavior is also responsible for enlarging the atomic holes observed after the melting process of the material. This happens because of the oxidation process in its surface.

The process of thermal treatment does not reduce the defects of surface, but causes electron dispersion in the net. Therefore, it can be considered an important factor for the catalytic reactions. When temperature is close to zero, a residual appears among electrons of the quasicrystal grouping. As a result, the disorders in the quasicrystalline net are impurities and vacancies.

For quasicrystalline materials can be applied Boltzmann transport equation in which the resistivity of material at low temperature can be described according to the following equation [6]:

$$\rho(T) = \rho_o + A.\Delta T^n \quad (1)$$

The above equation written in terms of conductivity gives:

$$\sigma(T) = \sigma_o + \sigma_o^{\,2}.\Delta T^n \quad (2)$$

In equation (2) σ and ρ are conductivity and resistivity, respectively; η depends on the type of dispersion (in this case $\eta = 2$ or electron – electron and $\eta = 3$ to 5 for electron – phonon) and A is a positive constant. The terms ρ and σ are physical characteristics related to dispersion mechanism with vacancies created in the thermal treatment process. This mechanism originates gaps and pseudogaps in the electron – electron interaction of the quasiperiodic structure [7].

3. THEORY OF GROUPING MODEL IN FERMI SURFACE

The model describes the formation of periodical and non periodical structures with forbidden allowed symmetries. In crystalline and quasicrystalline materials, an electron wave function is defined as [8]:

$$\psi(\vec{r}) = \mu(\vec{r}).e^{(i\vec{k}.\vec{r})} \quad (3)$$

In the above equation $\Psi\ \overrightarrow{(r)}$ is the wave function; $\mu\ \overrightarrow{(r)}$ is the reduced mass of a quasicrystalline net structure, $\overrightarrow{\imath k}$ is the wave vector and $\vec{r}$ is the unitary vector.

This function explains the symmetries of electron propagation in the net as well as the quantum transport of energy fulfilling the equation of Schrödinger given by [9]:

$$-\frac{\hbar^2}{2m}.\overrightarrow{\nabla}^2\psi(\vec{r}) + V(\vec{r}).\psi(\vec{r}) = E.\psi(\vec{r}) \quad (4)$$

where,

$\hbar^2$ represents the Planck constant, $\overrightarrow{\nabla}^2$ is a laplacian operator; m is the mass of system, $\psi(\vec{r})$ is the wave function of the electronic system, $V(\vec{r})$ is a potential function for the quasicrystalline net and E is the energy of the quasicrystalline structure.

In quasicrystalline structures the model applies the concept of state density defined as N(E) dE and the cluster model of the Fermi surface, can be used to study the adsorption and transport of solid surfaces or catalysts, which can describe the electronic density of states and transitions of alkali metals, used within the active sites of substrates. ; i.e., the number of autostate per unit of volume of an electronic system for a given direction of spin with energies E, described by the following equation [10]:

$$E_{Ft} = \int_0^{N_o} E(n).dN = \frac{3}{5}N_o.E_F \quad (5)$$

where the Fermi energy of the surface is,

$$E_F = \frac{\hbar^2}{2m}\left(\frac{3..\pi^2.N}{V}\right)^{2/3} \tag{6}$$

the final calculation of the total energy of the Fermi surface quasicrystal is:

$$E_{Ft} = \int_0^{N_o} \frac{\hbar^2.\pi^2}{2mL^2}.\left(\frac{3.N}{\pi}\right)^{2/3} dN \tag{7}$$

Once the Fermi energy is the total surface,

$$E_{Ft} = \frac{3^{5/3}.\pi^{4/3}.\hbar^2}{10m.L^2}.N_o^{5/3} \tag{8}$$

During the process for melting a quasicrystalline alloy, the temperature T of the set of electrons in the energy interval such as dE for each direction of spins in the structure causes modifications in the net. The function $f(E)$ describes a population of energy density as a function of Fermi distribution in quasicrystalline groupings. Equation for this function is given by:

$$f(E) = \frac{1}{e^{\frac{(\varepsilon_i - E_F)}{k_B T}} + 1} \tag{9}$$

where: ε_i is the energy in the i-th state; E_F is the potential energy of the Fermi surface; T is the temperature; k_B the Boltzmann constant. Figure 2 describes the distribution below the Fermi a function of temperature, temperatures employed in states with higher solids.

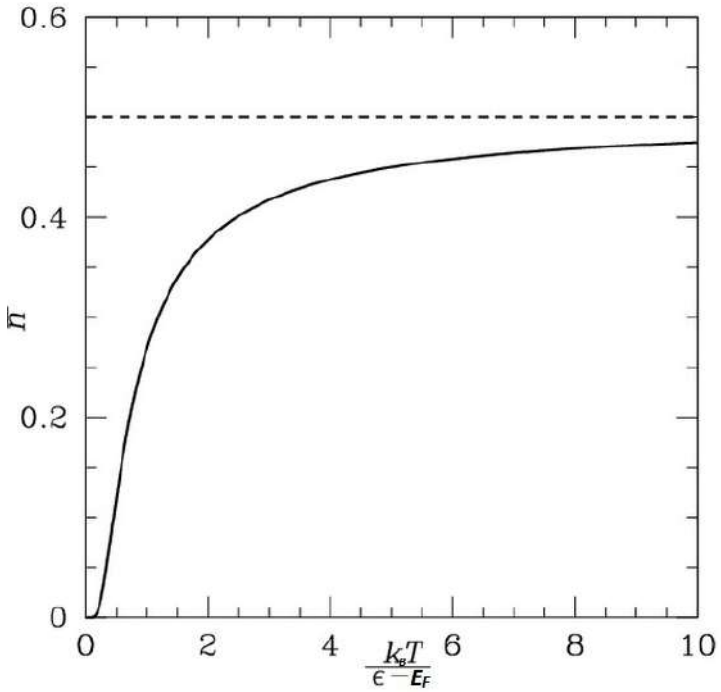

Figure 2. Fermi distributions function of temperature, temperatures employed in states with higher for solids.

The physical interpretation of the solids at low temperatures, the Fermi distribution is a step function that is 1 if $\varepsilon_i < E_F$ and 0 if $\varepsilon_i > E_F$. This means that the particles will be positioned from the lower energy level to above due to the Pauli Exclusion Principle have been made until all particles [11]. The energy of the last occupied level is called the Fermi energy and the temperature that corresponds to this energy by:

$$E_F = K_B.T_F \tag{9}$$

the Fermi temperature. If the condition that the Fermi temperature of most metals is great actual (approximately 10^3 K), therefore the approximation to say that the Fermi distribution remains a scalar to room temperature, which is valid with high precision. The Fermi statistical distribution is most commonly used to study the transport behavior of electrons in crystalline and quasicrystalline solids.

Calculations of *N (E)* and its correspondent auto functions for a quasiperiodic net are carried out according to the following approaches:
(1) The first approach considers the approximation of the free electron in the quasicrystalline net as a weak electronic dispersion in which its energy can be described by the equation:

$$E = \frac{\hbar^2.k^2}{2.m} \tag{6}$$

where, k is the wave vector and *m* is the effective mass of the quasicrystalline structure.

In this case, Fermi surface is spherical and has density of states given by each direction of spin of the system structure due to the approximation of the free electron in the quasiperiodic net. *N (E)* is now defined as follows [12]:

$$N(E) = \frac{\frac{4.\pi.k^2}{8.\pi^3}}{\frac{dE}{dk}} = \frac{m.k}{2.\pi^2.\hbar^2} = \frac{(m^3.E/2)^{1/2}}{\pi^2.\hbar^3} \qquad (7)$$

(1) In the second approach, both quasicrystalline and crystalline net are considered ideal. In these nets, phonons or impurities or other centers of dispersion introduce a kind of defect in the quasicrystal grouping. Therefore, it can be seen as free medium way such as L that distributes the electron propagation in Fermi surface.

In this approach, electron interactions with the centers of dispersion are analyzed. Furthermore, it is observed that these interactions modify the quasicrystal structure, its groupings and the electron transportation in its surface next to Fermi energy. It is also observed the creation of states "in loco" which define the insulator or the metallic behavior of crystalline and quasicrystalline materials.

The presence of centers of dispersions influences the grouping movement of the free electrons. This movement is observed when they are submitted to fields of temperatures which are created in thermal treatment. Hence, the net vibrations and defects are created at quantum level spreading the electrons in the quasicrystalline net.

Figure 3 illustrates two types of situations for weak electric field of ionic nature for quasiperiodic structure [13].

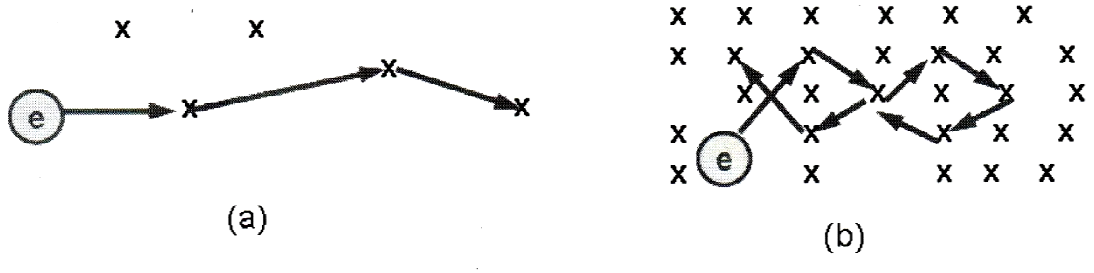

Figure 3. Illustration of two types of situations of weak electrical field of ionic nature for quasiperiodic structure (a) small dispersion center in the net and (b) concentrated dispersion center in the net.

Figure 3(a) shows that the centers of dispersion are few and do not influence the trajectory of electron in the net. In Figure 3(b), it is observed an increase of the concentration of dispersion in the net which change the trajectory of electron in the presence of external changes of ionic origin. As a result of the increase in concentration of dispersion, closed trajectories of electrons in Fermi surface in quasicrystals are observed. Therefore, it was created localized states with finite states densities limiting the wave function in an overposition in the structure rotations. In this figure the collisions do not influence significantly the movement of electrons

in the quasiperiodic net. Due to this behavior, it is not observed any deviation from its trajectory when in movement influenced by temperature or by external electric field.

The model analyzes this case as a diffusion of classic particles around the grouping of quasicrystal and applies the Boltzmann equation giving by:

$$\sigma = \frac{n.e^2.\tau}{m} = \frac{e^2.n.D}{E_F} \tag{8}$$

where, σ is the classical diffusion coefficient, n is the concentration of the population of particles (electrons), τ is the time of medium free way, m is the effective mass of grouping in quasicrystal and E_F is the Fermi energy in the surface "e".

The diffusion coefficient D is defined as follows:

$$D = E_F.L \tag{9}$$

where, V_F is the velocity of Fermi surface and L is the free medium way.

The diffusion process may create gaps due to Fermi energy or even pseudogaps due to density of states. Thus it is created a cohesive energy that justifies the mechanism of grouping in quasicrystals with its stability in quasiperiodic net [12]. When L is small and $kL > 1$, the changes in density of states are not big. Considering that quasicrystalline materials are amorphous, the disorder of electrons dispersion is responsible for its free medium way. The origin of quantum interferences of the wave functions for these materials is a good pioneer in chemical liaisons and in the quasicrystalline arrangements.

4. CONCLUSIONS

Grouping Model describes the behavior of groupings in quasicrystalline structures as well we the breakage of symmetry due to factors such as temperature, electric field and electric dispersion in the net. The latter explains the diffusion process of electrons on Fermi surface by the density of states of free electrons via Fermi Statistics.

The Boltzmann transport influences the temperature and resistivity propagation as, for example, the conduction of electrons in the quasicrystalline structure in the league formation process.

The long thermal treatment shows a tendency for creating significant vacancies. It is understood that there is no diminish in the surface defects but a material sinterization with non adequate thermal treatment. This creates quantum interferences in the centers of dispersions originating gaps and pseudogaps of energy next to Fermi surface.

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