

# PSEUDO-PERIOD OF DISTORTED LATTICES IN DISORDERED SOLIDS

M. A. GRADO-CAFFARO\* and M. GRADO-CAFFARO

*C/Julio Palacios 11, 9-B, 28029-Madrid (Spain)*

*(Received 17 January 1999; In final form 5 March 1999)*

Disordered lattices are discussed in terms of the spacing between adjacent atoms. This discussion is based on the randomness of the above spacing and on the crystalline potential by assuming a one-dimensional solid. Our theoretical considerations are useful to study certain aspects of amorphous semiconductors.

*Keywords:* Disordered lattices; spacing between adjacent atoms; amorphous semiconductors

## 1. INTRODUCTION

Analytical approaches to the study of disordered solids by using advanced tools of mathematical physics are really necessary since a considerable lack of knowledge on the above subject is due to the utilization of obscure techniques which are called by certain authors empirical techniques. As an example of mathematical-physics based methods for analyzing theoretically amorphous structures, we can mention Ref. [1]. In the same way as Ref. [1], we shall comment in the following certain aspects related to the randomness of the spacing between adjacent atoms in a distorted lattice; in particular, considerations upon crystalline potential will be made.

---

\*Corresponding author.

## 2. THEORY

First of all, we recall the following well-known fact: a solid in crystalline state presents a constant spacing between adjacent atoms; this spacing is the period of the corresponding crystalline lattice. In addition, it is also well-known that a given electron in the solid is submitted to a periodic potential so that the period of this potential is equal to the above spacing. The conception of this spacing as a random variable implies that the solid behaves as a disordered system. Then, for a disordered one-dimensional solid, we can write  $V(x+s) \neq V(x)$ , where  $V$  denotes potential energy,  $x$  is spatial coordinate (cartesian coordinate), and  $s$  stands for lattice period. The parameter  $s$  may be regarded as a random variable [1, 2]. Now, by considering the mean value theorem, we have ( $s$  can be regarded as a pseudo-period):

$$\begin{aligned} V(x+s) &= V(x) + s \left[ \frac{d}{dx} (V(x)) \right]_{x \rightarrow x+\theta s} \\ &= V(x) - sF(x+\theta s) \quad (s_1 \leq s \leq s_2)(0 < \theta < 1) \end{aligned} \quad (1)$$

but  $F(x+\theta s)$  represents the magnitude of the force acting on a given electron submitted to a lattice field whose corresponding potential energy is  $V$ . On the other hand, we can do the following reasoning: since crystallinity involves periodicity of  $V$  with a strictly fixed period, the magnitude of the quantity  $sF(x+\theta s)$  constitutes a measure of disorder so that, if this magnitude is relatively small, we can claim that the system in question presents a state relatively close to the crystalline phase. Therefore, minimization of the above magnitude corresponds to a quasi-crystalline state.

Another alternative picture of the situation in question should consist of considering a first-order Taylor expansion of  $V(x+s)$ , namely:

$$V(x+s) \approx V(x) - sF(x) \quad (s_1 \leq s \leq s_2) \quad (2)$$

However, the approximate formula (2) is only valid for relatively small  $s$ -values, that is to say, for  $s \ll d$  where  $d$  stands for the period of the crystalline lattice counterpart (see Ref. [1], p. 215). By virtue of this

ref., we have:

$$\int_{s_1}^{s_2} sx(s)ds = d \quad (3)$$

where  $x(s)$  is the probability density function of  $s$  as a random variable. At this point, by taking into consideration the probability interpretation of standard quantum mechanics,  $x$  is a random variable so  $x + s$  is another random variable whose probability density function should be a useful tool for examining complex situations. Finally, we want to remark that, by taking into account expression (2), quasi-crystalline systems correspond to a minimal  $F(x)$  so that one has  $V(x + s) \approx V(x)$ , as expected.

### 3. CONCLUDING REMARKS

In the previous brief study, we have called  $V$  the crystalline potential (potential energy corresponding to the crystalline state); in reality, this potential should be called potential of disordered lattice. In addition, we wish to emphasize that randomness is a crucial concept in our context so that complex situations in physics of amorphous materials can be studied by using special tools [1, 3] which, to date, have not been employed in the current literature. In particular, statistical concepts and sophisticated methods of signal theory and theory of dynamical systems should be used in this context.

#### *References*

- [1] Grado-Caffaro, M. A. and Grado-Caffaro, M. (1998). *Act. Pass. Electronic Comp.*, **21**, 213–215.
- [2] Grado-Caffaro, M. A. and Grado-Caffaro, M. (1998).
- [3] Franks, L. E., *Signal Theory* (Prentice-Hall, 1975).



**Hindawi**

Submit your manuscripts at  
<http://www.hindawi.com>

