

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).