

PSEUDO-PERIOD OF DISTORTED LATTICES IN DISORDERED SOLIDS

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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.

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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

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