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MEANING OF ENERGY DIAGRAMS USED TO DESCRIBE HETEROSTRUCTURES

by

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Abstract

Energy diagrams used to describe superlattices built by alternate doping are based on electrostatics, while those for heterostructures use potential barriers to simulate the effect of interferences produced by periodic potentials limited in space.

Key-words: Superlattices; Hererostructures.

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Since Esaki and Tsu[1] showed the feasibility of producing superlattice structures, the energy diagrams which they proposed to describe them are widely used to visualize and calculate a variety of physical situations[2].

In the case of superlattices built by alternate p-n-p-n-... doping, the conduction and valence bands of the host semiconductor are parallel (Fig. 1a), and their common slope at any place ℓ can be interpreted as an electric field $E(\ell)$ acting on the carriers (electrons and holes). The static field $E(\ell)$ arises from the uncompensated ionized donors and acceptors at the insulating junctions. This concept is used throughout in describing the functioning of devices based of p-n junctions[3].

In the case of superlattice heterostructures built with alternate layers of different semiconductors, the conduction and valence bands of the device are drawn in real space as to exhibit the different energy gaps of the constituent semiconductors and, therefore, the bands cannot be parallel everywhere. This is shown in Fig. 1b, for a superlattice composed by semiconductors with energy gaps Eg_1 and Eg_2; the smooth interpolations at the junctions describe a narrow region of graded energy gap which might result from a gradual change in semiconductor composition. In general, the relative energy distance of the conduction bands of the semiconductors has to be determined experimentally.

I would like now to call the attention to the fact that in the case of heterostructures the slopes of the conduction and valence bands at the interfaces are different, and thus, it is no longer possible to think in terms of an electric field. It would be physically inconsistent to associate an electric field to each slope since they are different

and, at the same time, they are supposed to act at the same place. It has been my experience that when this point is brought out, the reaction is one of surprise. Actually, the two cases are completely different and the proposed energy diagram for heterostructures requires some detailed justification.

First of all, I would like to emphasize that in contrast to the case of alternate doping superlattices, the energy diagram for heterostructures is not based on electrostatics.

It is well known that a periodic potential gives rise to an energy band structure; there is a certain energy range within which the carriers cannot propagate in the material (the forbidden energy gap). This results from a destructive interference of the carrier wavefunction in the periodic potential. Thus, a semicondutor behaves like a potential barrier to electrons with energies between the bottom of the conduction band and the top of the valence band, in the sense that they are reflected back if impinging on the semiconductor. If, however, the periodic potential is limited in space (thin semiconducting layer), there is a finite probability of tunneling through. It turns out that in the limit in which the transmission probability is small, the effect of the periodic potential can be fairly well simulated by a potential barrier where the carriers tunnel with an "effective mass" appropriate to the forbidden gap. This effective mass is obtained from the energy vs. wavevector relation for energies corresponding to the gap, where, of course, the wave vector is purely imaginary in this energy region. The details of the calculations for a one dimensional model are given in Ref. 4. Thus, the possibility of replacing a periodic potential limited in space by a potential barrier justifies the use of an energy diagram

of the type of Fig. 1b to describe heterostructures with thick enough semiconducting layers. Calculations using the true atomic potentials show that indeed the potential barrier approximation is not satisfactory for superlattices whose components have only a few ($\lesssim$10) monolayers[5]. Usually, these subjacent considerations are not explicitly stated when the superlattice energy diagram is used to visualize some physical process or to calculate the band structure of the superlattice.

In sum, the energy diagram of Fig. 1a is determined by the electrostatic charges of uncompensated donors and acceptors, while that of Fig. 1b describes an enterely different physical situation in which the effect of interferences within a periodic atomic potential is simulated by potential barriers.

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FIGURE CAPTION

Fig. 1 - Energy diagrams commonly used to describe superlattices. (d is the periodicity of the superlattice).

a) with alternate doping (host semiconductor with energy gap Eg), b) heterostructure with semiconductor gaps Eg_1 and Eg_2. Dotted lines show the slopes at position ℓ.

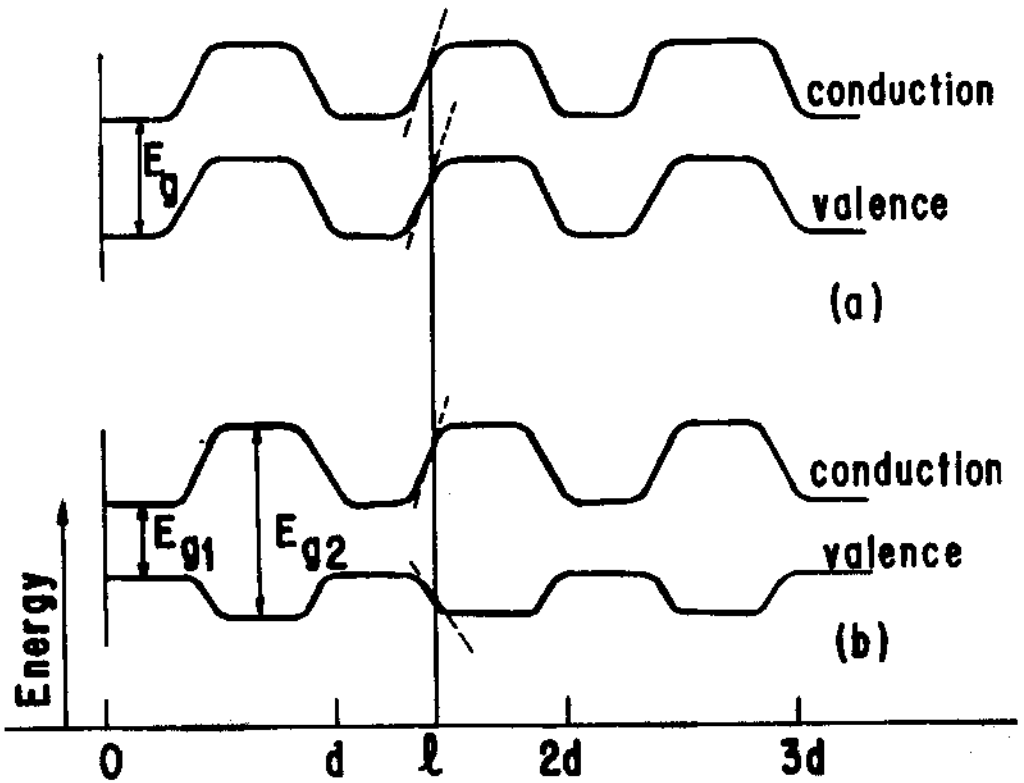
conduction
valence
(a)
conduction
valence
(b)
E_g
E_{g1}
E_{g2}
Energy
0
d
ℓ
2d
3d

Fig. 1

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