Quantum Size Effects and Localization Lengths in Disordered Heterostructures

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Many bulk polymers are semiconductors having tunable electronic properties as a function of composition. This variation in composition induces disorder. One of the main interests in these materials is the fact that the disorder showing correlations leads to the appearance of mobility edges in the density of states. In this work we explore this correlated disorder effects to build a one-dimensional model for heterostructures where quantum size effects are investigated when mobility edges are inherently included. Although heuristic, such a model represents an important step in understanding quantum well structures based on amorphous semiconductors or the recently proposed polymer based structures.

A number of disordered one dimensional (1D) systems, exhibiting nontrivial extended states, have recently been investigated theoretically[1]. It has been shown that the delocalization of states is a consequence of correlations imposed on the disorder[2]. These results are of paramount importance, since it has been believed for a long time that 1D disordered systems show only localized states[3]. Besides that, these localization effects are relevant for some models handling with the transport properties of some polymers (polyanilines)[4]. The prototype example of the situation where delocalization of states in 1D disordered chains occur can be summarized as follows. Considering a binary random alloy, whenever the bond between one of the atomic species is inhibited, one introduces a short range order that leads to the formation of a band of delocalized states. In other words, this effect occurs when, in a chain of A and B type sites, only A-A and A-B nearest neighbors bonds are allowed. Variations of this kind of correlations have been discussed in the literature recently, like the random dimer model. Here we are discussing the electronic properties of a linear chain treated in the tight-binding approximation, considering one s-like orbital per atomic site and nearest neighbor interactions only.

An important subproduct of these systems is the possibility to study localization versus quantum confinement effects. One can build up a quantum well with a finite segment of a linear disordered chain with this kind of correlation in the disorder. Since there are energy ranges showing either localized and delocalized states, one can directly monitor the spatial quantization as a function of the localization of the bulk states of the quantum well material. Although still a one-dimensional model, this approach goes one step further in investigating size quantization effects in disordered heterostructures, since now mobility edges of the "bulk chain" are inherently included.

The tools use in our work are the calculation of transmission probabilities and localization lengths, as well as the local density of states (LDOS). We begin by "characterizing" finite disordered linear chains with correlated disorder connected to ordered semi-infinite contact chains. This is the ideal configuration (finite segments connected to ordered contacts) to obtain informations on the electronic structure via the transmission probability of the finite chain segment considered. The method to calculate the transmission probability of this system, starting from a tigh-binding Hamiltonian

$$\mathcal{H} = \sum_n \epsilon_i |n><n| + \sum_n V_{n,n+1} |n><n+1| \ , \quad (1)$$

is described elsewhere[5]. The parameters used are: $\epsilon_A = 0.3$ eV, $\epsilon_B = -0.3$ eV, V_{AA}= 0.8 eV, V_{AB}=0.3

eV and V_{BB}= 0.5 eV. An important quantity to characterize the delocalization is the localization length[6], obtained from the transmission probability:

$$\lambda(\epsilon) = -\frac{2L}{\ln[T(\epsilon)]} \qquad (2)$$

where L is the length of the chain and $T(\epsilon)$ the transmission probability.

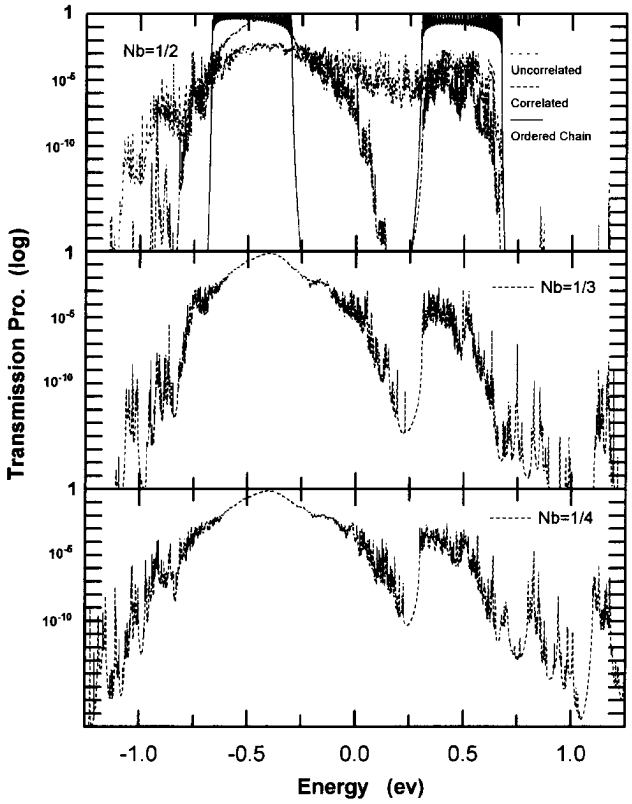

Figure 1. Transmission probabilities as a function of energy. The chains are 80 atomic sites long. Solid line represents the ordered chain. Doted lines denote chains with uncorrelated disorder. Dashed lines denote chains with correlated disorder.

In the Fig. 1 we show the transmission probabilities for chains with different concentrations of B-type sites (N_B), which are compared with the ordered chain for $N_B = 1/2$. The chains are 80 atomic sites long. We compare for $N_B = 1/2$ the uncorrelated and correlated disorder situations. From this figure it is clear that the correlation in disorder leads to the formation of delocalized states. The position in energy of the extended states is independent of the concentration of B-type sites. This result apparently indicates that the delocalization is due to a short range order introduced by the correlation.

From the same figure we can see that disoredered chains with correlation have a memory of at least two bands of the ordered systems. On the other hand, the uncorrelated case shows no delocalized states and has no memory of the bands for the ordered situation. The localization length reduces very fast when the correlation disappears, and increases when the B-type sites concentration reduces. In Fig. 2 we follow the localization lengths of the electronic states as a function of energy, and we can see clearly the delocalization of states as function of the correlation for different concentrations of B-type sites. Comparing Figs. 1 and 2 we see that the transmission probabilities show a smooth behavior when the localization length is of the order or longer than the chains considered.

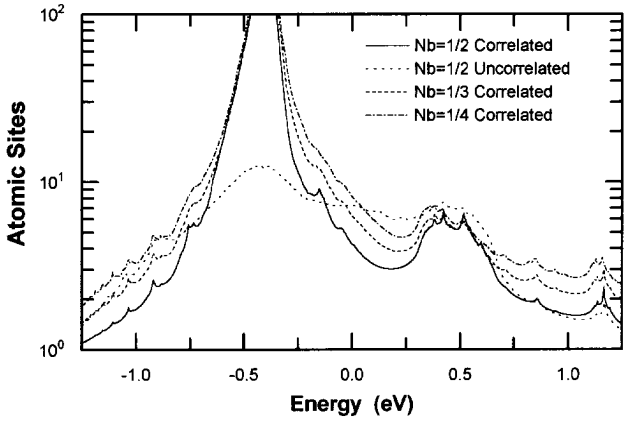

Figure 2. Localization length of wave functions as a function of energy for the same disordered chains of Fig. 1.

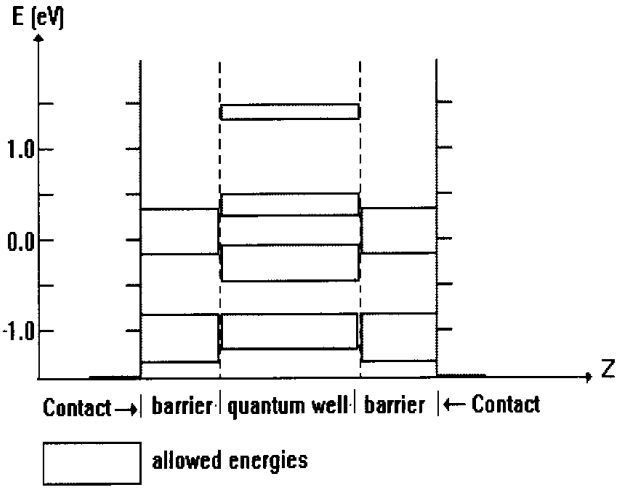

Figure 3. Scheme of the bands structure of a double-barrier quantum well for the ordered case. Barriers are 20 atomic sites long and the well has 36 atomic sites.

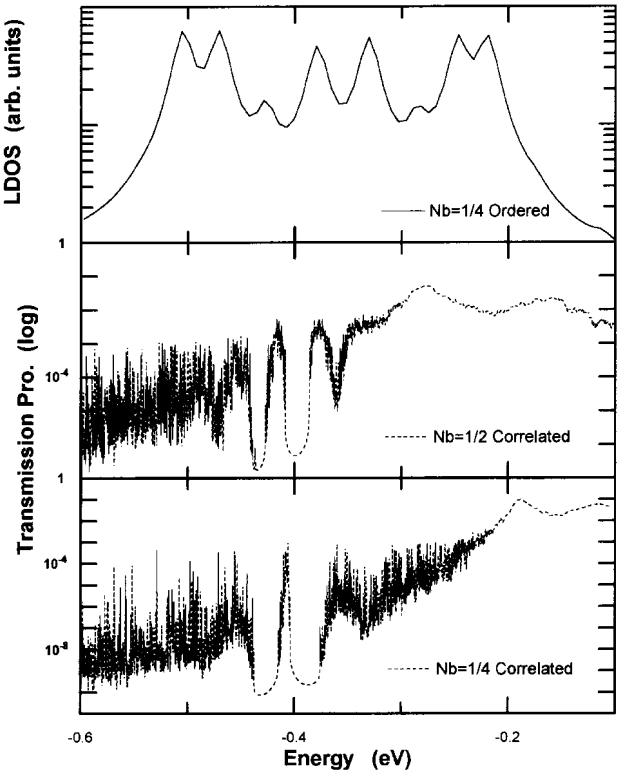

Figure 4. Top: Local density of states at a site in the well of a double-barriers structure. The ordered quantum well is 36 atomic sites long for the $N_B = 1/4$ case. Center and bottom: Transmission probabilities as a function of energy for disordered quantum wells.

We proceed by using the $N_B = 1/2$ and $N_B = 1/4$ chains with *correlated disorder* to build a quantum well. Fig. 3 shows the band structure profile used for the ordered case. The barriers are 20 atomic sites thick and the well is 36 sites wide. We consider disorder only in the quantum well. One should remind that the disorder modifies the local density of states. In the top of Fig. 4 we have the LDOS at a site in an ordered well of $N_B = 1/4$ type. The peaks can be identified with the size quantization levels. The two lower panels of Fig. 4 show the transmission probabilities for the barrier-QW-barrier configuration. One clearly observe resonances in the transmission probabilities. This resonances are due to the formation of quasi-bound states in the well due to size quantization. This can be verified by comparing the position in energy of the resonances with the position of these states in the LDOS (not show here).

It should be stressed that the resonances in transmission probability are only built-up when the localization lengths of the "bulk" states from the quantum well are longer than the thickness of the double-barriers structure considered. This point is made clear in Fig. 5, where we show the corresponding results to Fig. 4 *without correlation in the disorder*. We summarize our results by stabilishing that quantum size effects in disordered systems are possible. The necessary condition is that the localization lengths of the well material at energies where the quantum well levels should exist are longer than the device (double- barriers structure) considered.

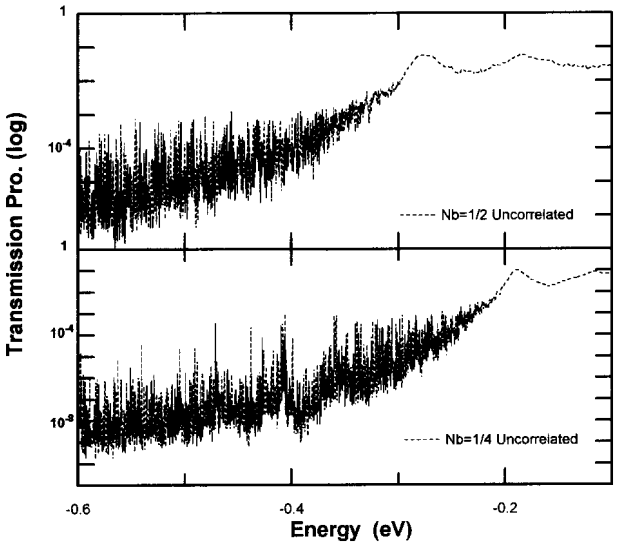

Figure 5. Transmission probabilities as a function of energy for quantum wells with uncorrelated disorder for different b-type sites concentration.

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