Electronic Properties of Compositionally Disordered Quantum Wires

J. P. G. Taylor,[1] K. J. Hugill,[1,2] D. D. Vvedensky,[1,2] and A. MacKinnon[1]
[1]*The Blackett Laboratory, Imperial College, London SW7 2BZ, United Kingdom*
[2]*Interdisciplinary Research Centre for Semiconductor Materials, Imperial College, London SW7 2BZ, United Kingdom*
(Received 26 December 1990)

Electronic states in quantum wires are studied using computer simulations of the growth to characterize the compositional disorder and a tight-binding Hamiltonian to determine the electronic densities of states. Calculations for monolayer slices of wires generated from the statistics of the simulated wires reveal the degrading effect of interface profile fluctuations and islands on the ideal quasi-one-dimensional electronic characteristics. Fixed-width fluctuations of the wire profiles, on the other hand, have a relatively minor effect on the first few subbands. Calculations of the localization length are used to characterize the mobility within the quantum wires.

PACS numbers: 73.20.Dx, 68.55.−a, 71.20.−b

The fabrication of semiconductor heterostructures by molecular-beam epitaxy (MBE) and related growth techniques has had an immediate and far-reaching impact on fundamental investigations and practical device development. Increasingly, attention is moving away from quasi-two-dimensional simple quantum wells and multiple quantum wells towards quasi-one-dimensional structures and networks of such structures, which may be grown by a variety of methods.

A natural extension of standard MBE growth on nominally flat surfaces is the growth on slightly misoriented (−2°–4°) surfaces of structures where the quantum confinement of carriers occurs in two dimensions, i.e., quantum "wires." The misorientation produces a sequence of alternating steps and terraces, with the important features for quantum wires being that growth occurs by step advancement [1] and that the same relative amount of the two materials is grown at each monolayer. This procedure has been applied with conventional MBE [2], migration-enhanced epitaxy (MEE) [3], and metal-organic chemical vapor deposition (MOCVD) [4].

There is a variety of reasons for studying the electronic properties of semiconductor quantum wires. The suggestion of a high mobility due to strong suppression of elastic scattering, by analogy with quasi-two-dimensional high-electron-mobility transistor (HEMT) structures, has led to the expectation that quantum wires could be used in high-speed electronic devices [5]. Furthermore, the laser characteristics of quantum-wire lasers have been predicted to show a significant improvement on those of quantum-well lasers in terms of threshold current, modulation dynamics, and spectral properties, provided there is no strong coupling among neighboring wires [6]. On a more fundamental level, quantum wires provide an opportunity to study electronic transport in ordered and disordered quasi-one-dimensional systems with some control over the lateral dimensions. This approach would complement previous work on molecular and polymeric chains, on the one hand, and metal wires and structured gate systems, on the other.

Implicit in many of the predicted characteristics of narrow quantum wires [6–8] is the assumption that the compositional disorder at the interface is either unimportant or can be controlled. When fabricated lithographically, the lateral dimensions are still large enough (>1000 Å) that the interface fluctuations are relatively unimportant, but produce only a limited separation of subband energies, so in most cases the broadening of the levels has been greater than the separation. Evidence for the presence of wire structures produced by direct growth methods has come from photoluminescence excitation studies, which show a strong anisotropy [3] in the intensity ratio of the electron–light-hole and electron–heavy-hole exciton peaks, depending on the orientation of the incident light polarization with respect to the direction of the quantum wires. However, the laser characteristics of these structures are not significantly better than lasers made from quantum wells with equivalent alloys. This is explained as being due to coupling between the wires and the roughness of the wire boundaries.

In this Letter, we examine the effects of compositional disorder on the electronic densities of states and localization lengths of simulated quantum wires. Our results provide the first clear indication of the effects of various types of disorder on the electronic states in quantum wires. Although quantum wires are not usually fabricated with MBE, the breakdown of the effects of various types of compositional disorder has implications for the electronic behavior of quantum wires fabricated by other techniques. Furthermore, only for conventional MBE are the details of the growth process known with any certainty, though models have been advanced for both MEE [9] and MOCVD [10].

In the solid-on-solid model of MBE [11], the substrate is modeled as a simple cubic lattice on which overhangs are not permitted. Growth is initiated by the random deposition of atoms onto the lattice at a rate JA, where J is the flux and A is the substrate area. The migration of adatoms is treated as a nearest-neighbor hopping process, with the hopping rate given by $k(E,T)=k_0\exp(-E/$

k_BT), where k_0 is an adatom vibrational frequency ($\approx 10^{13}$ s^{-1}), k_B is Boltzmann's constant, T is the substrate temperature, and E is the barrier to migration. The barrier consists of a substrate term E_S and a contribution E_N from each nearest neighbor along the substrate. Thus, $E = E_S + nE_N$, where $n = 0, 1, \ldots, 4$. By direct comparison with the experiments of Neave *et al.* [1], the optimum values of these diffusion barriers for GaAs(001) for the growth conditions of Ref. [1] have been determined to be $E_S = 1.45$ eV and $E_N = 0.3$ eV [8]. This allows a direct relation to be established between the simulated and experimental temperature scales, as described in Ref. [8].

Following previous work [12], we shall simplify the problem of quantum-wire growth by considering a system in which the two components of the quantum wire have identical kinetic properties and are differentiated solely by a label. In this way we can focus upon the influence of the growth kinetics in determining the electronic character of the structures. This procedure is necessitated in part by there being no systematic experiments of the type reported by Neave *et al.* [1] from which to estimate the kinetic parameters for Al during the growth of AlAs. Growth was simulated on a 120×80 lattice with four steps of terrace width equal to 20.

The electronic structure of the quantum wires was calculated using a tight-binding Hamiltonian, which allows the disorder at the interface to be treated exactly [13]. For the calculations reported here, we considered a single-band model with only nearest-neighbor interactions, though neither these approximations nor the use of a simple cubic lattice are intrinsic restrictions of the model. Our effective Schrödinger equation can be written in terms of site components as $\epsilon_i c_i + \sum_j V_{ij} c_j = E c_i$, where c_i is the amplitude of the wave function at site i, and ϵ_i is the potential, which takes either the value ϵ_{Ga} or ϵ_{Al}. The hopping elements V_{ij} are the kinetic-energy terms, which will be taken to have the constant value V between nearest neighbors and zero otherwise. For GaAs/AlAs wires, we must choose $\epsilon_{\mathrm{Al}} \gg \epsilon_{\mathrm{Ga}}$. In the limit $\epsilon_{\mathrm{Al}} \to \infty$, the Ga subband can be studied by considering only the Ga sites. This provides a considerable saving in the computer time and has little effect on the results when compared with more realistic values for ϵ_{Al}. It must be stressed, however, that this treatment is not intended to represent in detail any realistic GaAs/AlAs system, but only to treat on a quantum-mechanical level a system for which the *scattering* structure is similar to that of a realistic system.

Since we wish to compare the spectrum of the disordered wire with that of a perfect wire, we must perform the calculations with sufficient resolution to be able to resolve the important spectral features. A perfect wire of cross section $M \times M$ has a band of total width $12V$ containing M^2 subbands and $2M^2$ inverse square-root singularities. Thus each feature is of order $6V/M^2$. If fifty energy points are needed to span each feature adequately, then an energy step of order $\Delta E \approx V/8M^2$ is required. Now if a finite system of length L is considered, then the number of states in the spectrum is equal to the number of sites, i.e., $M \times M \times L$, and the average number of states in an interval ΔE is $N = M^2 L \Delta E / 12V \approx L/100$. For a reasonable representation of the density of states, approximately 200 states per energy interval are needed, implying a typical system length of $L \sim 20000$ sites. Since it is impractical to carry out the growth simulations with $L \sim 10^5$, we must adopt an alternative strategy.

We consider, as an initial calculation, wires with a one-dimensional cross section, which saves computer time without sacrificing the essential physics. Furthermore, submonolayer structures similar to those whose electronic structure we are calculating have been grown by MBE [14], so this idealization is not as drastic as it may first appear. Since the calculation of the density of states and the localization length employs an algorithm based on a recursive method for building up the wire slice by slice, it is desirable for our algorithm for generating the structure to work in a similar way. To characterize the compositional disorder of the simulated structures, the interface fluctuations and the island structures found within the wires are treated independently. Additionally, all islands of wire material outside of the main body of the wire were removed. These small structures cannot support states near the band edge and so are not important. With these approximations, the fluctuations of the two edges can be described in terms of two components, the meandering of the wire, represented by the fluctuation of the mean position of the two edges $\bar{y}$, and the fluctuation of the width of the wire Δy.

We anticipate, in the light of recent results on ballistic transport in split-gate structures [15], that the long-range variations in $\bar{y}$ and Δy will be much less important than the short-range behavior, and that the width fluctuations will be more important than the snaking. Our algorithm must therefore be designed to reproduce the short-range variations in the wire width as accurately as possible [16]. We use the distributions for the changes in $\bar{y}$ and Δy, $\mathrm{Prob}(\delta\bar{y})$ and $\mathrm{Prob}(\delta\Delta y)$, from which random values of $\delta\bar{y}$ and $\delta\Delta y$ can easily be chosen by a Monte Carlo procedure. By concentrating on these changes, we correctly reproduce the short-range behavior of the wire structure, while detailed balance should guarantee a reasonable reproduction of the absolute values of y_1, y_2, and Δy. The concentration of islands of Al within the simulated wires and the distribution of their sizes were analyzed and the generating algorithm was modified to include such structures. The concentration of these Al sites was estimated to be $q = 0.05$ for wires of width 10 and $q = 0.03$ for width 15. There was, however, a significantly higher fraction of larger Al islands in wires of width 15.

A comparison of generated and simulated structures is shown in Fig 1, including the successive incorporation of fixed-width fluctuations, or meandering [Fig. 1(a)], fluctuations in the width [Fig. 1(b)], and islands [Fig. 1(c)]

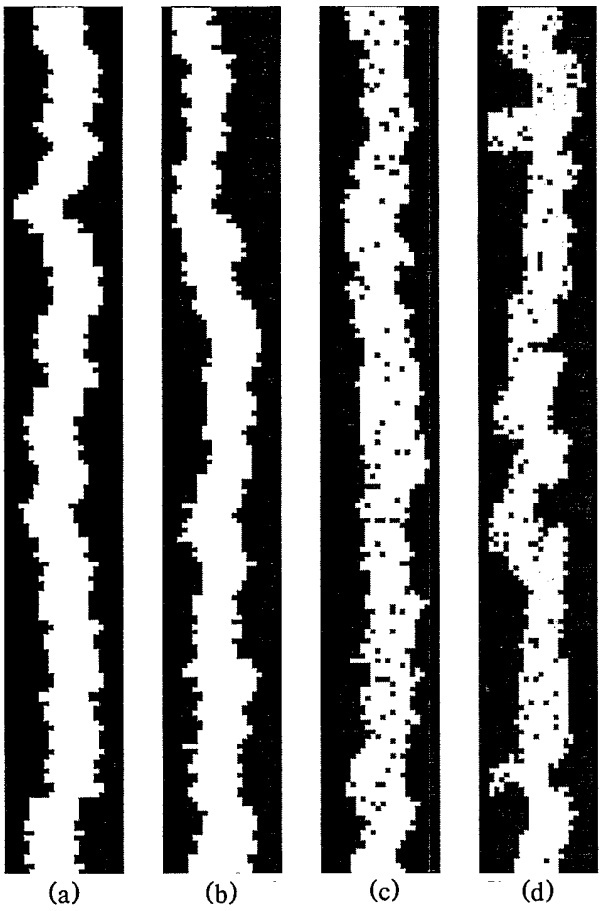

FIG. 1. Sections of the quantum wires of width 10 considered in the density-of-states and localization-length calculations: (a) fixed-width fluctuations with no islands (snaking); (b) including width fluctuations, but no islands; (c) including both width fluctuations and islands; (d) as in the growth simulations.

in generated wires, compared with a simulated wire [Fig. 1(d)]. The mean width in all three cases is 10 atomic units and the statistics used to generate these structures were taken from the appropriate correlation functions of simulated wires [Fig. 1(d)].

The integrated density of states was calculated using a method revived by Evangelou [17] and based on the work by Dean and Martin [18]. The densities of states near the band edge for the generated wires in Figs. 1(a)–1(c) are shown in Fig. 2. The physically interesting region of the spectrum is that close to the band edge, where the wave functions with long wavelengths along the wire direction should be least sensitive to perturbations of the wire width. The effect of meandering on the density of states is quite small and is not shown. However, the inclusion of width fluctuations has an evident detrimental effect, with only the first subband having a sharp definition (Fig. 2, curve *b*). The addition of islands has an even stronger degrading effect (Fig. 2, curve *c*), presumably by forcing nodes in the wave function, which wipes away the

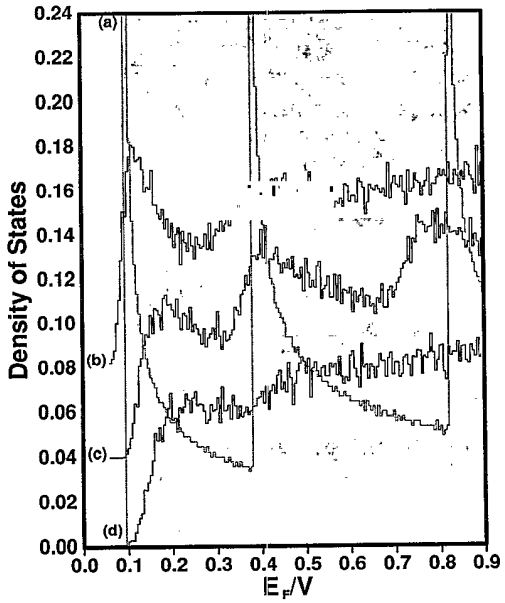

FIG. 2. The density of states of various width-10 wires (solid lines, curves *b*–*d*) plotted alongside the ordered case (dotted line, curve *a*). Curve *b*, fluctuating width without islands; curve *c*, fixed width with islands; curve *d*, fluctuating width with islands. Curves *c* and *d* have been shifted vertically.

remaining characteristic features of the density of states. Note in particular that the broadening due to width fluctuations seems to increase with increasing energy, whereas the effect of islands is roughly energy independent.

These results can be understood using simple arguments. If the energy of the quantized levels in a system of width L is $E \sim n^2/L^2$, then the fluctuation of the energy is roughly $\delta E \sim E(\delta L/L)$, which is a strong function of the width L. On the other hand, the coherent-potential approximation for the islands yields a self-energy $\Sigma = -q/G$, where q is the density of islands defined above and G is the Green's function on a single site. This is not very dependent on the level index and leads to an energy-independent broadening.

As a result of the random fluctuations of the width, there is a finite probability that the wire structures being generated will be broken at some length. The occurrence of such breaks will have a drastic effect on the transport capabilities of the wires. For the electronic model used here such a cut would result in the electrons in the total wire having zero mobility. Using the generating algorithm discussed above, the average length before such a break is found to be [16] ~20000 slices without islands and ~5000 slices with islands. For a system with a full two-dimensional cross section the typical wire length would be expected to be an order of magnitude greater than this.

Whether or not the wire structures are connected over long distances in a quantum-mechanical sense can be in-

vestigated by calculating the transmission probability T. Because all states are localized exponentially in any one-dimensional disordered system [19], we can define a localization length λ for a system of length L by $T = \exp(-2L/\lambda)$. This localization length, which is the appropriate definition of the quantum-mechanical connectivity of the wires, was calculated using the well-tried transfer matrix method [20,21]. Each point was generated using systems corresponding to ~ 50000 slices, i.e., $\sim 5\%$ error. The results show that the disorder is sufficient to localize all of the states to well within the classical length of the wire, the systems without islands having a typical localization length of ~ 90 lattice units and the system with islands, of ~ 30 lattice units. Hence, contrary to the predicted high mobility for idealized wires, the simulated wires will in fact have very low mobility.

The results presented here show that the densities of states and electron mobilities of monolayer wires grown on vicinal surfaces by conventional MBE deviate drastically from those determined on the basis of ideal structures. This is in stark contrast to the behavior found for quantum wells, for which sharp spectra and high mobilities are now achieved routinely even for relatively narrow wells. Nevertheless, our data contain strong indications that if island formation is suppressed then the definition of the first few subbands would be substantially improved, which holds promise for optical applications of quantum wires. Studies that go beyond monolayer structures will be required to assess the prospects for electronic transport applications of quantum wires.

The support of the Science and Engineering Research Council (United Kingdom) and Philips Research Laboratories Redhill, United Kingdom, are gratefully acknowledged.

[1] J. H. Neave, P. J. Dobson, B. A. Joyce, and J. Zhang, Appl. Phys. Lett. **47**, 100 (1985).
[2] P. M. Petroff, A. C. Gossard, and W. Weigmann, Appl. Phys. Lett. **45**, 620 (1984).
[3] M. Tsuchiya, J. M. Gaines, R. H. Yan, R. J. Simes, P. O. Holtz, L. A. Coldren, and P. M. Petroff, Phys. Rev. Lett. **62**, 466 (1989).
[4] T. Fukui and H. Saito, Appl. Phys. Lett. **50**, 824 (1987).
[5] H. Sakaki, Jpn. J. Appl. Phys. **19**, L735 (1987).
[6] Y. Arakawa, K. Vahala, and A. Yariv, Appl. Phys. Lett. **45**, 950 (1984).
[7] H. Sakaki, Jpn. J. Appl. Phys. **19**, 94 (1980).
[8] M. L. Roukes, A. Scherer, S. J. Allen, H. G. Craighead, R. M. Ruthen, E. D. Beebe, and J. P. Harbison, Phys. Rev. Lett. **59**, 3011 (1987).
[9] Y.-T. Lu, P. Petroff, and H. Metiu, Appl. Phys. Lett. **57**, 2683 (1990).
[10] T. Fukui, H. Saito, and Y. Tokura, Jpn. J. Appl. Phys. **27**, L1320 (1988).
[11] J. D. Weeks and G. H. Gilmer, Adv. Chem. Phys. **40**, 157 (1979).
[12] K. J. Hugill, S. Clarke, D. D. Vvedensky, and B. A. Joyce, J. Appl. Phys. **66**, 3415 (1989).
[13] A. K. Myers-Beaghton, J. P. G. Taylor, D. D. Vvedensky, K. J. Hugill, and A. MacKinnon, J. Cryst. Growth **111**, 328 (1991).
[14] M. Tanaka and H. Sakaki, Appl. Phys. Lett. **54**, 1326 (1989).
[15] L. I. Glazman, G. B. Lesovik, D. E. Khmel'nitskii, and R. Shekhter, Pis'ma Zh. Eksp. Teor. Fiz **48**, 238 (1988) [JETP Lett. **48**, 258 (1988)].
[16] Note that this procedure does not remove any overhangs connected to the edge of the main wire section. However, we do not consider this to be a serious omission.
[17] S. N. Evangelou, J. Phys. C **19**, 4291 (1986).
[18] P. Dean and J. L. Martin, Proc. R. Soc. London A **259**, 409 (1960).
[19] N. F. Mott and W. D. Twose, Adv. Phys. **10**, 107 (1961).
[20] A. MacKinnon and B. Kramer, Z. Phys. B **53**, 1 (1983).
[21] J. P. G. Taylor and A. MacKinnon, J. Phys. Condens. Matter **1**, 9963 (1989).