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Simulation of multilayered resonant tunneling diodes using coupled Wigner and Boltzmann distribution function approaches

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From a coupling model between the Boltzmann transport equation and the quantum Liouville equation, we have developed a simulator based on the Wigner distribution function (WDF) approach that can be applied to resonant tunneling diodes (RTDs) and other vertical transport quantum devices. In comparison to previous WDF simulators, the tool allows one to extend the simulation domains up to hundreds of nanometers, which are the typical dimensions required for the study of actual multilayer structures. With these improvements, a level of agreement between theory and experiment comparable to that obtained by using other simulators based on Green functions has been achieved. The results of this work reveal that the WDF formalism can be alternatively used to study the behavior of actual multilayered RTDs. © *2000 American Institute of Physics.* [S0003-6951(00)05347-X]

Because of its high switching speed, low power consumption, and reduced complexity to implement a given function, resonant tunneling diodes (RTDs) have recently been recognized as excellent candidates for digital circuit applications.[1] In parallel to technological efforts aimed toward searching compact circuit architectures, a great deal of attention has been dedicated to model and simulate RTDs, as a way to optimize device design and fabrication,[2] and also to understand mesoscopic transport properties of these devices. In this regard, reliable transport approaches must include the main physical processes in the device (namely electron transmission, reflection, and scattering processes), as well as self-consistency and open system boundary conditions.

Quantum kinetic models, such as those based on the nonequilibrium Green function formalism, have been demonstrated to fit the previous requirements. Between them, the approach of Lake *et al.*[3] has recently gained increasing interest due to its ability to incorporate coherent and incoherent interactions in a unified formulation, as well as band structure. On the other hand, the Wigner distribution function (WDF) approach, obtained from the nonequilibrium Green function formalism by using the lattice Weyl transform,[4] has been extensively applied to the simulation of RTDs.[5–8] Although this formulation can be improved in some aspects (such as a treatment of carrier scattering more realistic than the usual relaxation time approximation), several works have demonstrated that the main physical phenomena expected for the devices (and related to quantum effects) are reproduced within the formalism. In this regard, it is worth mentioning the work of Jensen and Buot,[6] who simulated the intrinsic high frequency oscillations in current for a fixed bias voltage in the negative differential resistance region of the $I-V$ characteristic. However, to develop reliable simulators, not only qualitative, but also quantitative predictions of device behavior are required. To this end, it is necessary to consider simulation domains large enough to include the complex multilayer structure of actual devices. In previous works,[6–8] the CPU time associated with the iterative solution of the quantum Liouville equation has severely limited the spatial domains only to the double barrier region and adjacent layers of few tens of nanometers. Under these conditions, it is difficult to go beyond qualitative studies of RTD behavior. We have recently proposed a new WDF-based model for the simulation of RTDs, that allows one to extend the simulation domains up to several hundreds of nanometers without a significant increase in computational burden in comparison to previous tools.[9] Based on it a RTD simulator has been developed. The main purpose of this work is to demonstrate how our tool is able to reasonably reproduce the static $I-V$ characteristic experimentally measured in actual devices.

Our model is based on the coupling between the WDF transport equation (quantum Liouville equation) and the Boltzmann transport equation. The former is applied to the active region of the device including the double barrier and well, where quantum effects are present [we call this region the quantum window (QW)]. The latter is solved by means of a Monte Carlo (MC) algorithm and applied to the remaining portion of the device, where the potential profile varies smoothly and quantum effects are not expected to occur (details of coupling and ohmic contact boundary conditions are given in Ref. 9). Although the idea of separation into a quantum region and classical regions was already used by others,[10] it has never been previously applied to develop a simulator based on the WDF approach. Since the classical MC algorithm is much less time consuming than the WDF solver, the simulated classical regions can be extended up to several hundreds of nanometers without a significant increase in computing times. The width of the QW can be made variable, but we will use a value comparable to the length of typical simulation domains considered in previous tools based only on the solution of the Liouville equation. This ensures that a semiclassical approach can be applied beyond the QW boundaries. To achieve self-consistency, the Poisson's equation is iteratively solved in the whole device

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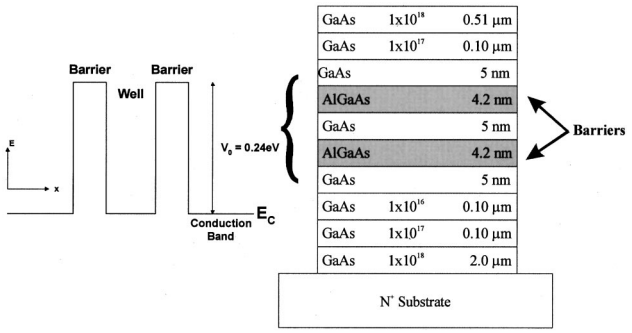

FIG. 1. Structure of the RTD under study (the device has been fabricated at the University of Leeds by P. Steenson). To optimize computer time, the first highly doped AsGa buffer layer (2 μm) on top of the substrate has been discarded. This has little effect on simulated results since current level is mainly controlled by the doping of the inner layers.

with the Liouville/Boltzmann equation in the quantum/classical regions for each applied voltage. The number of steps is chosen to guaranty that current convergence is achieved at the end of each iterative procedure. Finally, the relevant magnitudes for device simulation, i.e., electron concentration and current density, have been obtained in each region (QW and classical regions) from the corresponding distributions (WDF and MC) according to standard expressions.[5,11]

The previous model has been successfully used to simulate the behavior of RTDs with different physical parameters.[12] Continuity of charge density and electrostatic potential at the QW boundaries has been obtained, and the main qualitative features expected for the devices have been reproduced from the simulations. However, we have not yet compared simulated results with experimental data. This has been difficult so far since the multilayer structure of actual devices requires the consideration of simulation domains much larger that those achievable with previous WDF-based tools. To demonstrate the potentiality of our tool, we have carried out the simulation of the $I-V$ characteristic of the RTD shown in Fig. 1 (simulation parameters similar to those of Ref. 12 have been used). The result is shown in Fig. 2 together with the experimentally measured $I-V$ curve. Good prediction of resonant and valley voltages is obtained from

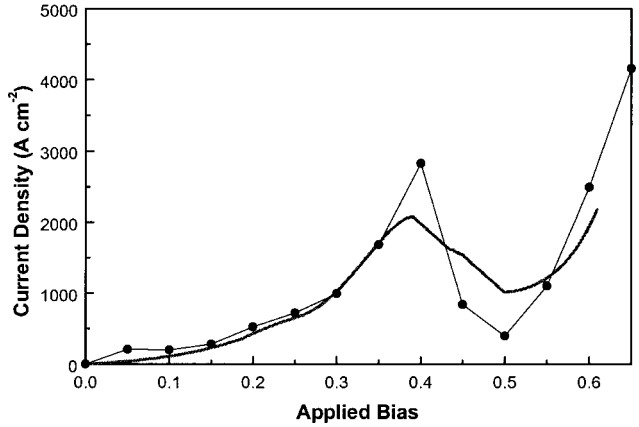

FIG. 2. Comparison of the simulated (dots) and experimental (continuous line) $I-V$ curve of the RTD of Fig. 1. The barrier height has been slightly modified from the nominal value to fit the measured characteristic. The experimental $I-V$ curve is due to P. Steenson and has been used with permission of the author.

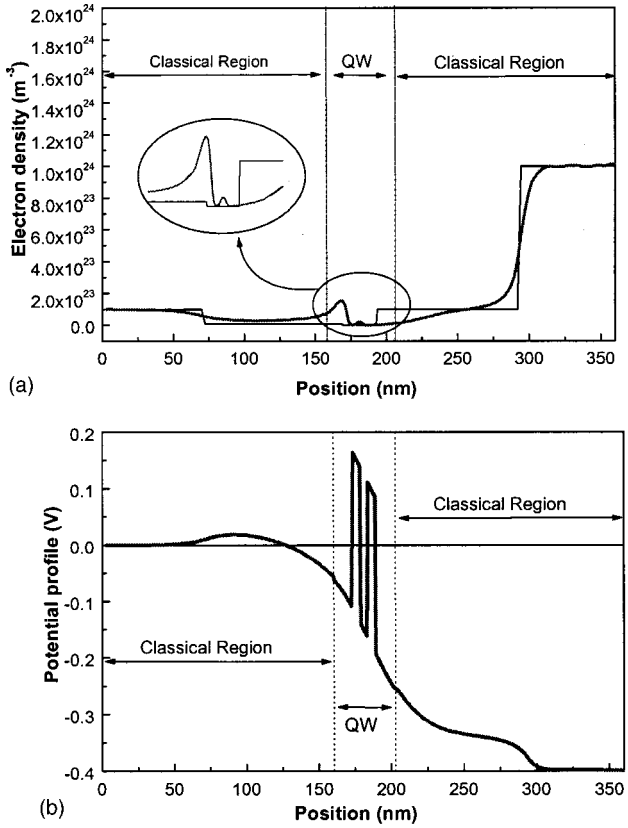

FIG. 3. Simulated electron density (a) and potential profile (b) for the device of Fig. 1 under resonance (0.4 V). For comparison, doping density is also depicted in (a). A significant electronic charge accumulates in the well at this applied bias (inset).

the simulator. Due to the exponential dependence of current on barrier geometry (width and height) and to tolerance of physical parameters, it has been necessary to allow a slight deviation of one physical parameter (barrier height) from the nominal value to achieve a good fit. A barrier height of 0.27 eV (which lies within the expected tolerance for this parameter) has been used to obtain the simulated $I-V$ characteristic of Fig. 2. To determine this parameter we have fitted the pre-resonance portion of the $I-V$ curve, since for voltages above resonance intervalley transitions can be important and these have not been modeled in our simulator. In fact, this can be the reason that explains why the peak-to-valley ratio is overestimated by our simulator. Figure 3 shows the simulated electron density and potential profiles for an applied bias of 0.4 V (resonance). In view of Fig. 3 it is clear that simulation domains as short as the QW width (which are the typical box dimensions considered in previous tools based only on the WDF) are not suitable to obtain reliable results, since charge neutrality (or flatband condition) is not obtained at the extremes of the QW boundaries. This is mainly due to the relatively small doping level of those layers adjacent to the undoped spacers, which is also the origin of the considerable potential drop in the emitter. As in previous simulations, the results of Fig. 3 exhibit good matching at heterojunctions, homojunctions, and QW boundaries.

Theoretical and measured characteristics do not exactly match (the simulator fails in correctly predicting the experimental peak-to-valley current ratio), but resonant and valley bias are acceptably estimated. In our opinion, the level of

agreement between theory and experiment is comparable to that obtained by means of the Green function approach (NEMO program[10,13,14]). Certainly, one parameter has been slightly modified from the nominal value to achieve the fit presented in Fig. 2. As stated in a recent paper,[14] growth related uncertainties may lead to discrepancies between theory and experiment; therefore, some degree of freedom is necessary to fit simulated and experimental results. Specifically, in Ref. 14 significant discrepancies between experimental results and those calculated by means of the NEMO program using nominal parameters are apparent. The authors attribute the underestimated peak bias and current to small differences between designed and as-grown physical parameters. Being that the barrier width of devices considered in Ref. 14 is as thin as 2 nm (which corresponds to few monolayers), it is not surprising that there is a mismatch between the measured resonant voltage and the value predicted by the simulator. The device simulated in the present work has a double barrier region considerably wider. Therefore, better accuracy in layer widths is expected. This may be the reason why our prediction of peak bias satisfactorily matches the experiment. However, it is likely that the Al mole fraction in the as-grown AlGaAs layers does not perfectly coincide with the design value. Since current is very dependent on barrier height (and hence on Al mole fraction), it is not surprising that the value that better fits the experimental $I-V$ curve (0.27 eV) presents a small shift as compared to the design value (0.24 eV). However, this difference is very small and lies within the limits of tolerance for barrier height. In our opinion, accurate predictions of experimental $I-V$ curves in RTDs require not only reliable transport models, but also precise control on as-grown parameters. The level of agreement between design and as-fabricated parameters will have direct influence on the success in correctly predicting device behavior. Nevertheless, simulation tools for actual devices are useful to analyze the effects of physical parameters on transport properties, and also to extract design guidelines. In this regard, this work shows that our WDF-based tool can be considered as an alternative to other well-developed simulators to the study of RTDs.

In conclusion, it has been demonstrated that our tool, based on the WDF formalism, allows one to simulate actual RTD device structures. Although improvements can be made, the obtained results show promise to use our simulator as a tool to guide in RTD device design. It can also be used to study electronic transport properties of quantum mesoscopic devices with core regions sandwiched between large classical domains.

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