Random impurity and phonon-scattering processes in multibarrier structures

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In mesoscopic devices, in addition to the tunnel barriers, the electrons interact with a random configuration of impurities as well as with phonons. The scattering processes are usually modeled using (a) Matthiessen's rule with (b) phenomenological parameters. In this paper, we investigate the validity of such scattering models and propose an alternative approach based on the Keldysh formulation and the diagrammatic analysis. Consequently, the scattering rates depend on the strength of the disorder, the temperature, the electron energy as well as on the spatial coordinates. However, we show that the semiclassical Matthiessen rule can be used to combine the two scattering rates in quantum effect devices assuming large electron mean free paths and within the scope of self-consistent Born approximation. The assumption of a large mean-free path remains valid for moderately strong disorder even at room temperature, which makes our model suitable for practical simulation of electron transport. [S0163-1829(97)07407-9]

It is well known that quantum-mechanical models, based on pure or coherent quantum states,[1–3] alone cannot describe the carrier transport mechanisms in nanostructure devices, e.g., the resonant tunneling structures. This is because phase-breaking and inelastic-scattering processes influence the transport processes in these devices.[4] To include the effects of various scattering processes, most transport models use a phenomenological constant imaginary potential, a constant mean-free path, or a constant phase-breaking time.[5–9] When more than one type of scattering is present in a device, Matthiessen's rule (the scattering rates simply add) is commonly used to combine these scattering processes. Such models, while attractive, are not always adequate to describe nonequilibrium transport in mesoscopic devices. Klimeck *et al.*[9] have aptly shown that although inclusion of inelastic scattering is necessary for realistic simulation of quantum effect devices, use of phenomenological scattering rates inside the active devices does not guarantee current continuity. For these reasons, some attention has been given to develop rigorous transport models for various scattering processes.

The effects of inelastic scattering in disordered mediums have been studied widely in reference to the localization problem (for a review, see Ref. 10). It is known that random impurity scattering processes do not destroy the phase coherence of the two sets of time-reversed paths around the impurities interfering at the starting point (electrons and holes moving in opposite directions around the loop). The effect of such constructive interference, known as the weak localization, leads to decreased conductivity. On the other hand, electron-phonon interaction tends to destroy the phase coherence between the time-reversed paths and decreases the phase-coherence length. Consequently, the circumference of the loops of paths, which contribute to weak localization decreases, and the effects of weak localization gets weaker at higher temperatures. Moreover, it has been shown that even in quasi-one-dimensional semiconductor wire nanostructures, localization is unlikely to affect device performances; hence its effect can be neglected for such devices operating at elevated temperatures.[11] In three dimensions, states are not localized for weak disorder, and localization effects are much less pronounced on the transport properties.[12]

In this paper, the nonequilibrium Green's-function technique (Keldysh formalism)[13] is used for a rigorous description of the scattering rates in mesoscopic devices. In our model, to guarantee the conservation of charge and current continuity, the scattering rates become functions of both the energy and the position coordinates. The electron scattering rates due to phonons and impurities are added using Matthiessen's rule. Although Matthiessen's rule is derived semiclassically, one generally expects it to remain valid even for mesoscopic devices when the scattering rates are low enough. However, we report the results of an investigation into the regime of validity for the application of Matthiessen's rule in such devices when electron-random impurity (disorder) and electron-phonon scattering processes are considered.

To simulate the electron-random impurity scattering, we use a model that was developed recently.[14] It was shown in that model that the self-energy, resulting from the ensemble averaging, leads to phase breaking of the electron waves. The impurity potential in our model is uncorrelated and very short ranged and is described by a Gaussian white-noise model. The Green's function of our interest needs to be averaged over the ensemble of random impurities.[15] The general term in the perturbation series of the Green's function involves a very large number of possible diagrams. To sum the series, we use the Born approximation in which only two scatterings from a single impurity are considered. The expression for τ_{imp} is as follows:[14]

$$\frac{1}{\tau_{\mathrm{imp}}(\mathbf{r};E)} = \frac{2\pi}{\hbar}\, n_0 V_0^2 N_0(\mathbf{r};E). \tag{1}$$

Here, n_0 is the density of the impurities, V_0 is the impurity potential, and $N_0(\mathbf{r};E)$ is the local position-dependent density of states (DOS).

The electron-phonon scattering is described via a model developed by Datta.[16] The phonons are represented by a bath of independent oscillators within the harmonic approxima-

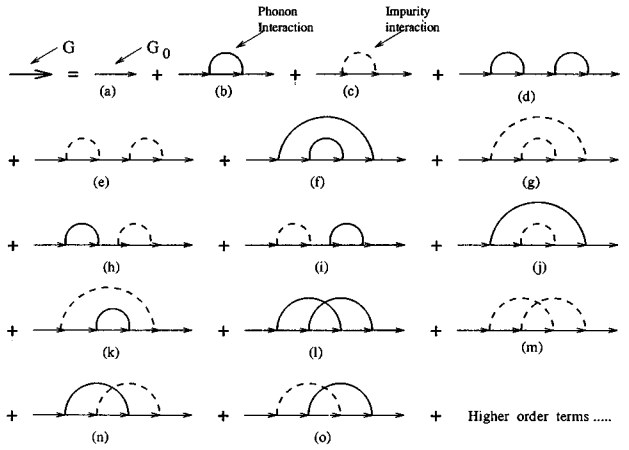

FIG. 1. The series of the Green's function up to second-order terms in the presence of both random impurity and phonon interactions.

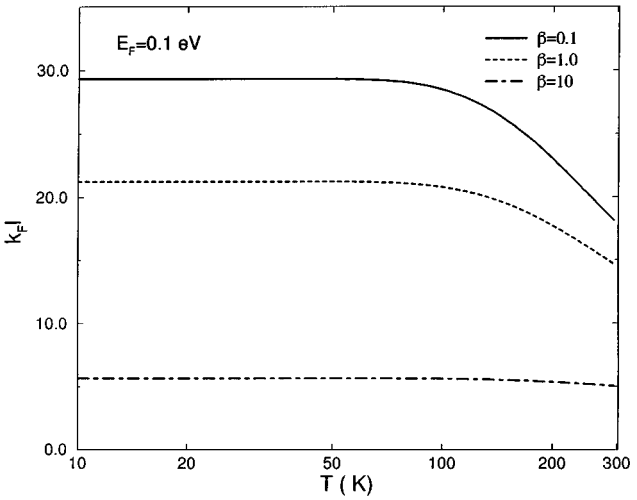

FIG. 2. Plot of $k_F l$ vs T with β as the parameter.

tion. Each oscillator interacts with electrons through a delta-function potential in space. The expression for τ_{phon} is given by Datta:[16,17]

$$\frac{1}{\tau_{\text{phon}}}=\frac{1}{\tau_{p_{\text{phon}}}}+\frac{1}{\tau_{n_{\text{phon}}}}, \tag{2}$$

where

$$\frac{1}{\tau_{p_{\text{phon}}}}=\frac{2\pi}{\hbar}\int dE' F(\mathbf{r};E')N_0(\mathbf{r};E-E')f(\mathbf{r};E-E') \tag{3}$$

and

$$\frac{1}{\tau_{n_{\text{phon}}}}=\frac{2\pi}{\hbar}\int dE' F(\mathbf{r};E')N_0(\mathbf{r};E+E')[1-f(\mathbf{r};E+E')]. \tag{4}$$

$f(\mathbf{r};E)$ is the local electron occupation factor and is given by

$$f(\mathbf{r};E)=\frac{1}{N_0(\mathbf{r};E)}\frac{\hbar}{2\pi}\int d\mathbf{r}'\,\frac{|G^R(\mathbf{r},\mathbf{r}';E)|^2}{\tau_p(\mathbf{r}';E)} \tag{5}$$

with

$$F(\mathbf{r};\hbar\omega)=U^2 J_0(\mathbf{r};|\hbar\omega|)\times\begin{cases}N(\hbar\omega) & \text{if } \omega>0\\ N(|\hbar\omega|)+1 & \text{if } \omega<0\end{cases}$$

and G^R is the retarded Green's function.

To combine the above-mentioned scattering rates, we begin with the Green's function for the device in the presence of scatterings from both phonons and random impurities. Considering only one phonon event, the series of the Green's function up to second-order terms is shown in Fig. 1. Note that the Feynman diagrams for the Green's function contain two types of diagrams. In one type, the impurity or the phonon interaction lines do not intersect one another. The other type consists of intersecting interaction lines. It is known that the contributions from diagrams with intersecting interaction lines are $(k_F l)^{-1}$ times smaller than those with no intersecting interaction lines.[18] Here k_F is the electron Fermi wave vector and l is the mean-free path in the presence of scattering from both random impurities and phonons. Thus for $k_F l \gg 1$, one neglects the diagrams with intersecting interaction lines [terms like (j) through (o) in Fig. 1] and sum up the remaining diagrams. The resulting Dyson equation,

$$G=G_0+G_0\Sigma G, \tag{6}$$

contains a self-energy term Σ given as $\Sigma=\Sigma_{\text{phon}}+\Sigma_{\text{imp}}$. G_0 is the noninteracting Green's function and G is the Green's function in the presence of both types of interactions. It is important to note that the above-mentioned self-energy terms are no longer independent of the other; each of these must now be evaluated using the total Green's function in a self-consistent manner. To estimate Σ_{imp} and Σ_{phon} in the coordinate space, we use the following expressions:[18]

$$\Sigma_{\text{imp}}=n_0 V_0^2 G(\mathbf{r}_1,\mathbf{r}_2;t_1,t_2)\,\delta^3(\mathbf{r}_1-\mathbf{r}_2) \tag{7}$$

and

$$\Sigma_{\text{phon}}=D(\mathbf{r}_1,\mathbf{r}_2;t_1,t_2)G(\mathbf{r}_1,\mathbf{r}_2;t_1,t_2). \tag{8}$$

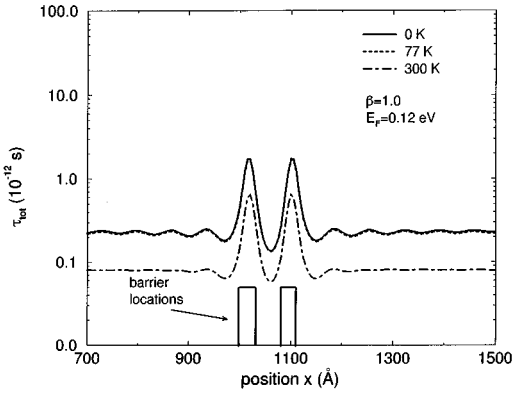

FIG. 3. τ_{tot} vs x for the same DBQW device as in Fig. 4 for three different values of T. $E_F=0.12$ eV and $\beta=1.0$.

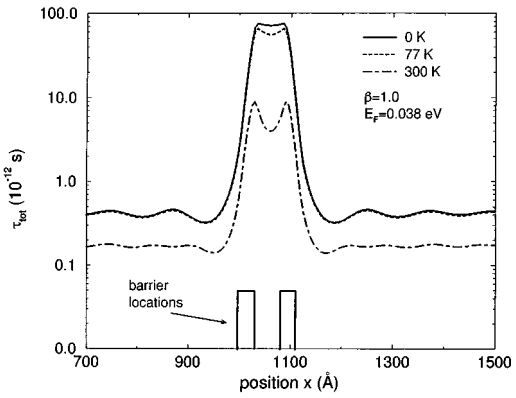

FIG. 4. τ_{tot} vs x for the DBQW device with T as the parameter. Here, $E_F=0.038$ eV such that $E_F+\hbar\omega_0<E_0$ and $\beta=1.0$.

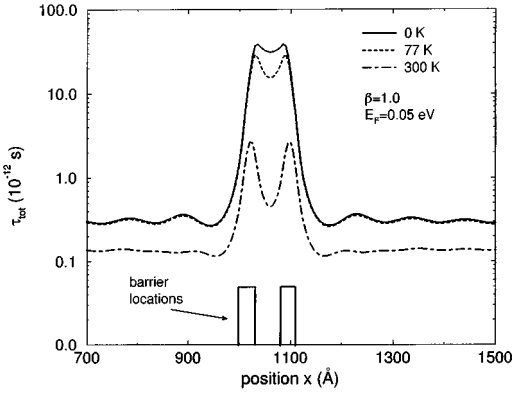

FIG. 5. τ_{tot} vs x for DBQW device for three different values of T. $E_F=0.05$ eV such that $E_F<E_0<E_F+\hbar\omega_0$. The value of $\beta=1.0$.

The consequence of expressing the total self-energy as a sum of the two components is that one can also express the total scattering rate as a sum of the two components. Finally we obtain

$$\frac{1}{\tau_{\text{tot}}}=\frac{1}{\tau_{\text{phon}}}+\frac{1}{\tau_{\text{imp}}}. \tag{9}$$

Here τ_{tot} is the total scattering time, τ_{phon} is the scattering time due to electron-phonon scattering, and τ_{imp} is the electron random-impurity scattering time. These scattering times are obtained from the imaginary parts of the respective self-energies. Thus one finds that the assumption of large electron mean-free path is necessary for the derivation of Matthiessen's rule for mesoscopic devices.

We now investigate the regime of validity of the basic assumption of our model, i.e., $k_F l\gg 1$. Here, $l=\tau_{\text{tot}}v_F$ and v_F is the Fermi velocity. For GaAs devices, optical phonons dominate the electron-phonon scattering processes. To estimate the electron-phonon scattering rate, within the harmonic approximation for the phonon spectrum, one needs to choose the electron-phonon scattering strength $[\propto U^2 J_0(\hbar\omega)]$.[16] We use the Einstein model for optical phonons where the phonon spectral density $J_0(\hbar\omega)\sim\delta(\omega\pm\omega_0)$, with $\hbar\omega_0=36$ meV. We have chosen a value of U such that Eq. (2) gives $\tau_{\text{phon}}=8\times10^{-12}$ s for the bulk GaAs at 77 K. The value of τ_{phon} used in our computation is also consistent[16] with that obtained in the semiclassical analysis based on Fermi's golden rule.[19] On the other hand, to quantify the strength of the disorder in our calculations, we have used a single dimensionless parameter defined by $\beta=3.24\times10^{66}n_0V_0^2$, where the dimensions of n_0 and V_0 are in SI units.[14] It is noted that, in bulk GaAs, the disorder of value β corresponds to a low-temperature mobility of $\mu\simeq(7000/\beta)$ cm^2/V s.

Figure 2 shows the plot of $k_F l$ vs T for various values of the disorder strength β with the Fermi energy $E_F=0.1$ eV. It is observed that for $\beta\leqslant 1$ (moderately strong disorder), our approximation remains valid even at room temperature. Note that, for such strengths of the disorder, the electron-phonon scattering processes are insignificant up to the liquid-nitrogen temperature (77 K). However, near $\beta=10$, the assumption of $k_F l\gg 1$ is not reasonable.

In Figs. 3–5 we present a pictorial summary of the effects of disorder parameter β, temperature T, the Fermi energy E_F, and the position x on τ_{tot} in a a double-barrier quantum-well (DBQW) device. The well of the device is 50 Å wide, and the barrier width and the height are 30 Å and 0.3 eV, respectively. The lowest resonant energy for this structure is $E_0\sim0.08$ eV. It should be mentioned that in the three-dimensional (3D) model of the DBQW, the 3D DOS inside the well is large for all energies $E>E_0$.

Figure 3 corresponds to $\beta=1.0$. The Fermi energy $E_F=0.12$ eV. Since $E_F-\hbar\omega_0>E_0$, electrons at this energy can both absorb and emit optical phonons. The figures show results at three different temperatures. We observe that τ_{tot} is dominated by disorder at 77 K and the effects of the phonons become substantial only near room temperature.

Figure 4 shows a similar plot for $E_F=0.038$ eV and $\beta=1.0$. The energy value was chosen such that $E_F+\hbar\omega_0<E_0$ and $E_F-\hbar\omega_0>0$ eV. Since the 3D DOS is low for $E<E_0$, the scattering rate $1/\tau_{\text{tot}}$ inside the well is about two orders of magnitude smaller than that shown in Fig. 3. In Fig. 5, we have used $E_F=0.05$ eV, which is also less than the resonant energy E_0. However, since $E_F+\hbar\omega_0>E_0$, the probability of phonon absorption is greatly enhanced due to the availability of a large DOS above the resonant energy.

In conclusion, we have presented a transport model for multibarrier mesoscopic devices that includes both electron-phonon and electron-random impurity interactions. The total scattering rate has been obtained from the Feynman diagrams of the Green's function using the Keldysh formalism. Our analysis is based on the assumption of large mean-free path of electrons. The regime of validity of our model has been investigated. It is shown that for typical moderately disordered systems, the theory remains valid even at room temperature.

Our calculations for DBQW devices show that the spatial variation of the scattering time can be quite large in multibarrier structures. Moreover, the scattering rate $1/\tau_{\text{tot}}$ is a function of disorder and temperature as well as of the electron energy. One of the attractive features of our scattering model is that our transport model always guarantees electronic-charge conservation and current continuity. The above is not true for the phenomenological scattering models.

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