OFFICE OF NAVAL RESEARCH

Grant N00014-90-J-1193

TECHNICAL REPORT No. 30

Escape Time From a Biased Asymmetric Double Quantum Well

by

Lakshmi N. Pandey and Thomas F. George

Prepared for publication

in

Journal of Applied Physics (Communications)

Departments of Chemistry and Physics
State University of New York at Buffalo
Buffalo, New York 14260

November 1990

Reproduction in whole or in part is permitted for any purpose of the
United States Government.

This document has been approved for public release and sale;
its distribution is unlimited.
11. TITLE (Include Security Classification)
   Escape Time From a Biased Asymmetric Double Quantum Well

12. PERSONAL AUTHOR(S)
   Lakshmi N. Pandy and Thomas F. George

13a. TYPE OF REPORT
13b. TIME COVERED
    FROM ___________ TO ___________
14. DATE OF REPORT (Year, Month, Day)
    November 1990
15. PAGE COUNT
    14

16. SUPPLEMENTARY NOTATION
    Prepared for publication in the *Journal of Applied Physics (Communications)*

18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
   DOUBLE QUANTUM WELL, ESCAPE TIME
   ASYMMETRIC, QUASIBOUND STATES, BIASED
   RESONANT TUNNELING

19. ABSTRACT (Continue on reverse if necessary and identify by block number)
   The escape time from the quasibound states of an asymmetrical structure consisting of a narrow well and a wide well separated by a relatively thick barrier under bias has been calculated. As expected, a monotonic decrease in the escape time from the ground state of the wide well as a function of applied voltage has been found. However, the variation of the escape times from the ground state of the narrow well and the first-excited state of the wide well versus applied voltage form a minimum at a common point. This is the signature of resonant tunneling when these two states almost coincide.
Escape time from a biased asymmetric double quantum well

Lakshmi N. Pandey and Thomas F. George
Departments of Physics & Astronomy and Chemistry
Center for Electronic and Electro-optic Materials
State University of New York at Buffalo
Buffalo, New York 14260

The escape time from the quasibound states of an asymmetrical structure consisting of a narrow well and a wide well separated by a relatively thick barrier under bias has been calculated. As expected, a monotonic decrease in the escape time from the ground state of the wide well as a function of applied voltage has been found. However, the variation of the escape times from the ground state of the narrow well and the first-excited state of the wide well versus applied voltage form a minimum at a common point. This is the signature of resonant tunneling when these two states almost coincide.

1990 PACS Nos.: 73.20.Dx. 71.50.+t. 73.60-n
How long it takes for a moving particle to tunnel through a potential barrier is a problem being investigated since the discovery of alpha particles. Recently, the interest in investigating the time scale involved in the tunneling process was revived after the work of Tsu and Esaki. Since then, the study of tunneling has opened a new field as far as physics and electronic devices are concerned. In the first study of the current-voltage (I-V) characteristic of a layered structure, a decrease in the current was observed as the potential difference increases. The explanation of this negative differential resistance (\( \frac{dV}{dT} \)) came from the resonant tunneling of carriers through the double barrier and a well system formed by thin layers of different semiconductors grown by molecular beam epitaxy (hence referred as a resonant tunneling structure, RTS). The static properties of RTS has been well investigated, and a list of recent developments in this area can be found in the book by Bastard. But the time taken by a carrier to complete the tunneling process in such structures is less studied. There are various definitions of this time scale available in the literature, and a complete list of these definitions and interdependences can be found in a review article by Hauge and Støveng, where they have tried to remove the interpretational controversy.

Recently, Oberli et al measured the resonance tunneling time in an asymmetric coupled quantum well under bias. Their structure consists of two wells of different thicknesses (narrow and wide, henceforth referred as NW and WW) coupled by a relatively thick barrier, implying that the two wells are loosely coupled. In the case of no external field, the states are localized either in NW or WW as if these wells were isolated. This fact could be demonstrated by looking at the localization of the eigenfunctions of the different states of the system. The changes brought by an external electric field are different for each state. For a given electric field, two of the states may coincide with each other. This particular case has been called the resonant tunneling. Oberli et al in their photolumi-
nescence experiment found that the tunneling time reduces to a minimum as the strength of the applied electric field increases, after which it tends to increase as the field continues to increase. This minimum tunneling time was found at the applied electric field strength for which the ground state of NW coincides with the first-excited state of WW. As the field increases from the resonance tunneling point, these resonant states become dealigned, causing delay in the tunneling process. Such a process was verified through photocurrent measurements.4

The experimental observation of Oberli et al4,5 was also verified theoretically through an ensemble Monte Carlo simulation,9,7 where polar optical phonon scattering, intervalley scattering, impurity scattering and electron-electron scattering are included explicitly. There have also been some attempts to calculate some time related physical properties of quantum structures, as described in Ref. 3.

In this present Communication, we calculate the escape time of the electrons from the quasibound states of an asymmetric coupled double quantum well under bias. A simple method is described to calculate the widths of the quasibound states, and hence from the uncertainty relation, the escape times of the electrons. The time calculated through this method cannot be compared directly with the experimental measurements of Oberli et al.4,5 but our results confirm the resonant tunneling process.

The bottom of the conduction bands of $Al_xGa_{1-x}As$ and GaAs forming the asymmetric double quantum well under forward bias are shown in the Fig. 1. Let us assume that the widths of NW, WW and the middle barrier are $d_n$, $d_w$ and $d_b$. The middle barrier and the left and right walls are formed by $Al_{0.3}Ga_{0.7}As$ providing a constant barrier and wall height, say $V_0$. The energy $E$ and position $x$ are measured from the middle of the structure where the applied field is zero. The boundaries of the structure are defined as $x_1 = -(d_n + d_w + d_b)/2$, $x_2 = (d_n - d_w - d_b)/2$, $x_3 = (d_n + d_b - d_w)/2$ and...
A general Schrödinger equation for a barrier or well region of the biased structure can be written by a simple coordinate transformation as

\[
\frac{d^2\psi_0[\rho(x)]}{d\rho^2} - \rho(x)\psi_0[\rho(x)] = 0 ,
\]

whose solutions are the Airy function \( Ai[\rho(x)] \) and its complement \( Bi[\rho(x)] \), and \( \rho(x) \) is the new coordinate system related to \( x \) by \( \rho(x) = -\alpha(m^*)[\pm x - \frac{\mathcal{V}}{eF}] \) with \( \alpha(m^*) = [2m^*/eFh^2]^{1/3} \). Here, \( F \) is the external electric field applied (normally measured in voltage per unit length), \( m^* \) is the effective mass, and the \( \pm \) sign refers to the forward and backward bias. These \( Ai(x) \) and \( Bi(x) \) are oscillatory for negative values of \( x \) and are complicated exponential functions for positive \( x \). Hence, the wavefunction in a region can be given as \( \Psi(x) = aAi[\rho(x)] + bBi[\rho(x)] \), where \( a \) and \( b \) are wavefunction amplitudes.

Following the matrix method, the amplitudes \( a_5 \) and \( b_5 \) in the region to the right of \( x_4 \) can be expressed in terms of \( a_1 \) and \( b_1 \) in the region to the left of \( x_4 \) as

\[
\begin{pmatrix}
a_5 \\
b_5
\end{pmatrix} = \mathbf{M}
\begin{pmatrix}
a_1 \\
b_1
\end{pmatrix},
\]

where \( \mathbf{M} \) is a 2 \( \times \) 2 matrix resulting from the boundary conditions (that wavefunction and its derivative divided by the effective mass of the region be continuous across the interface) expressed as

\[
\mathbf{M} = \mathbf{M}_{x_4}^{-1}(R)\mathbf{M}_{x_3}(L)\mathbf{M}_{x_3}^{-1}(R)\mathbf{M}_{x_2}(L)\mathbf{M}_{x_2}^{-1}(R)\mathbf{M}_{x_1}(L)\mathbf{M}_{x_1}^{-1}(R)\mathbf{M}_{x_1}(L).
\]

The subscripts on the matrices indicate the interface points, and \( L \) and \( R \) stand for the left and right of the interface. For example, the matrix of the region to the left of \( x_4 \) for a forward bias can be given as

\[
\mathbf{M}_{x_4}(L) = \begin{pmatrix}
\frac{Ai(\beta)}{\frac{m_4}{m^*}Ai'(\beta)} & \frac{Bi(\beta)}{\frac{m_4}{m^*}Bi'(\beta)}
\end{pmatrix},
\]

where \( \beta = -\alpha(m^*)[x_4 + \frac{E^*}{eF}] \), \( Ai'(\beta) = \frac{dAi(\rho)}{d\rho} \big|_{\rho=\beta} \), and \( m^*_4 \) is the effective mass of the electron in the region to the left of \( x_4 \). In the case of a forward bias as shown in the
Fig. 1. for the wavefunction to be bound, the amplitude $b_1$ must be zero, because as $x$ decreases in the region to the left of $x_1$, $Bi[\rho(x)]$ increases monotonically and tends to $\infty$. In the region to the right of $x_1$, the amplitude $a_5$ must be zero, giving rise to the condition for quasibound states of the system as $a_5 = M(1.1)a_1 = 0$. For all practical purposes, $a_1$ can be taken to be unity, although it can be found from the normalization condition, $\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1$. The quasibound states of the system can be found by finding the zeroes of the function $f(E) = M(1.1)$ by varying $E$. An analytic expression of $f(E)$ can be given in terms of the $A_i$ and $B_i$ functions calculated at the interfaces, but it is very lengthy and omitted for the purpose of this Communication. However, a numerical solution of $f(E) = M(1.1)$ can be found easily and accurately. All the matrices on the right-hand side of Eq. (3) are calculated numerically and multiplied together to find $M$.

The eigenvalues of the unbiased structure are stationary, whereas the applied field brings about a tilt in the barriers, such that these states are no longer stationary but are quasibound with a finite width and escape time. The amplitudes in the region to the right of $x_4$, $a_5$ and $b_5$ should provide the information about this width. Following Stone and Lee, and Price, it can be shown that the ratio $R(E) = \frac{a_5^2 + b_5^2}{a_5^2} = \frac{1}{1 + (E - E_h)^2/\Gamma^2}$ of the squares of the amplitudes of the wavefunctions in the regions to the left and to the right of $x_4$ is Lorentzian in the vicinity of the quasibound state energy $E_h$. This Lorentzian distribution can be expressed with the help of a Taylor series expansion of $a_5$ around $E_h$.

$$R(E) \simeq \frac{R_0(E_h)}{1 + (E - E_h)^2/\Gamma^2} \cdot$$

where $\Gamma = \frac{d}{dx} \frac{b_5(E_h)}{a_5(E_h)}$ is the width of the state and $R_0(E_h) = \frac{a_5(E_h)^2 + b_5(E_h)^2}{a_5(E_h)^2}$ is a constant for a particular quasibound state. The width of the quasibound state can be found by numerically differentiating $a_5$ with respect to $E$, and we can in turn find the escape time $\tau = \frac{4}{\Gamma}$ of the electrons from the quasibound state.

As mentioned earlier, the potential profiles of the bottom of the conduction bands
forming the narrow and wide wells separated by a barrier are shown in the Fig. 1. For illustrative purposes, the applied field strength has been taken to be 60 kV/cm. The widths of NW and WW are 60 and 88 Å, respectively. Three different widths, 40 and 55 and 65 Å, have been considered for the barrier which separates NW and WW. These width parameters are measures of the samples used by the Oberli et al. in their experiments. We have assumed that the barrier height \( V_0 \) is 65% of the total band-gap difference between GaAs and \( \text{Al}_x\text{Ga}_{1-x}\text{As} \). This difference has been calculated according to the expression given by Lee et al. \( \delta E(V_0/0.65) = 1.155y + 0.37y^2 \), where \( y \) is the Al fraction in AlGaAs. The effective mass of the electron in the different regions is derived by the expression \( m^* = 0.067 + 0.088y \).

For the set of parameters described above in the case of no bias, the three consecutive subbands of the structure have been found at 36.5, 60.8 and 148.8 meV, respectively, for the three values of the barrier widths. By looking at the localization of the eigenfunctions of these states (not shown here for brevity), one can conclude that the state at 36.5 meV is the ground state of WW, whereas the states at 60.8 and 148.8 are the ground state of NW and first-excited state of WW, respectively. The fact that the states are practically independent of the width of the barrier means, in the case of no bias, that the wells keep almost their own identity. This also implies that the two wells are very loosely coupled. Our result is in agreement with that of Ricco and Azbel \(^1^2\) quoted by Oberli et al. \(^4\) We would like to mention here once again that our zero of energy is at the origin of the spatial dimension.

In the case of a field of 60 kV/cm, there are three states situated at 4.8, 97.7 and 113.2 for a 40 Å barrier, at 0.33, 102.6 and 108.2 meV for 55 Å, and at -2.67, 104.5 and 106.3 meV for 65 Å. Figure 1 also displays the envelope functions of the three quasibound states of the structure considered here for the 55 Å barrier width. Our earlier statement
about localization of the eigenfunctions under no bias is clarified here in the case of a bias, such that the states are mostly situated in the either of the wells.

In Fig. 2 we show the variation of $\log_{10} R(E)$ as a function of the energy at the 60 kV/cm bias voltage and for the 55 Å barrier width. The ratio $R$ is distributed in a Lorentzian form in the neighborhood of the quasibound states. It is also clear that at the bias of 60 kV/cm, the ground state of NW is quite close to the first-excited state of WW. Our result for the energy and $\tau$ of the ground state of WW versus the bias voltage shows a constant decrease as the bias voltage increases, which is a consequence of the broadening of the ground state of WW and not shown here for brevity.

The change in the energy of $\nu$ and the escape time from the ground state of NW is shown by the solid lines, and for the first-excited state of WW is shown by the dashed lines as a function of applied voltage in Fig. 3 for the 55 Å barrier width. The energy of the ground state of NW increases as the bias voltage increases up to certain a point, and the energy of the first-excited state of WW decreases up to the same point. As mentioned earlier, this point is called the resonance tunneling point. For the parameters considered here, the resonance point is found, respectively, at 72.7, 64.0 and 59.4 kV/cm for the 40, 55 and 65 Å barrier widths. The value for the 55 Å barrier width is in agreement with that of Ricco and Azbel\textsuperscript{12} quoted by Oberli et al.\textsuperscript{4} These values are also in agreement with the expression of Oberli et al\textsuperscript{3} that the values of the applied voltage at which resonant tunneling takes place are given by $e|F| = \frac{2\Delta E}{d_n + 2d_s + d_w}$, where $\Delta E$ is the energy difference of the ground state of NW and the first-excited state of WW in the case of no bias, which is about 82 meV in our present case.

It is clear from Fig. 3 that the escape time $\tau$ of both states reaches a minimum at the resonance tunneling point and begins to rise for the field greater than the resonance tunneling point. While these two states are positioned close to each other in the neighbor-
hood of the resonance voltage, the minimum values of $\tau$ are different. These values of $\tau$ for the ground state of NW and first-excited state of WW for the 33 Å barrier are 87.04 and 55.34 ps. Resonant tunneling of an electron from one subband to another subband across a barrier is a coherent and elastic process. In other words, the barrier becomes transparent, and electrons see the whole structure instead of either well. This well broadening of the well causes an increase in the escape time in the vicinity of the resonance voltage. A usual decrease in the escape time as a function of the applied voltage has been found away from the resonance voltage. A similar behavior is also found for the other two barrier thicknesses.

In conclusion, we have presented a simple method to calculate the width of and hence, escape time from a quasibound state. The method involves the exact wave functions for the quantum-well structure under an external electric field, except for the numerical differentiation of the square of the amplitude of the wavefunction with respect to energy. We have calculated the escape times from the quasibound states of an asymmetric structure consisting of a narrow well and a wide well separated by a relatively thick barrier under bias. An expected monotonic decrease in escape time from the ground state of the wide well is found as a function of the applied voltage. The escape times from the ground state of the narrow well and from the excited state of the wide well versus applied voltage form a minimum at a common point, which has been called the resonance point. At this point the two states are in resonance, and hence the existence of the barrier separating the two states seems to have disappeared. The electrons sees the whole structure instead of either well alone, and the broader localization causes the delay in the escape.

This research was supported in part by the Office of Naval Research.
References


Figure captions

Fig. 1. Potential profiles of the asymmetric double quantum-wells system under bias. The narrow and wide wells are, respectively, 60 and 88 Å, being separated by a barrier of 55 Å. The solid, dashed and dot-dashed curves are the eigenfunctions of the first three eigenstates at a 60 kV/cm bias voltage.

Fig. 2. Log_{10} value of the ratio of the squares of the amplitudes of the regions to the left and to the right of \( x_4 \) \( R(E) \) at a 60 kV/cm bias voltage as a function of electron energy.

Fig. 3. Upper panel: subband energies of the ground state of NW (solid line) and first-excited state of WW (dashed line) versus the applied voltage for the barrier width of 55 Å. Bottom panel: escape times of the corresponding states.
Fig. 3

Pande and Geor
<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Address</th>
</tr>
</thead>
<tbody>
<tr>
<td>Professor John Baldeschwieler</td>
<td>Department of Chemistry</td>
<td>California Inst. of Technology, Pasadena, CA 91125</td>
</tr>
<tr>
<td>Professor John Eyler</td>
<td>Department of Chemistry</td>
<td>University of Florida, Gainesville, FL 32611</td>
</tr>
<tr>
<td>Dr. Sylvia Johnson</td>
<td>SRI International</td>
<td>333 Ravenswood Avenue, Menlo Park, CA 94025</td>
</tr>
<tr>
<td>Professor Paul Barbara</td>
<td>Department of Chemistry</td>
<td>University of Minnesota, Minneapolis, MN 55455-0431</td>
</tr>
<tr>
<td>Professor James Garvey</td>
<td>Department of Chemistry</td>
<td>State University of New York, Buffalo, NY 14214</td>
</tr>
<tr>
<td>Dr. Zakya Kafafi</td>
<td>Naval Research Laboratory</td>
<td>Washington, DC 20375-5000</td>
</tr>
<tr>
<td>Professor Stanley Bruckenstein</td>
<td>Department of Chemistry</td>
<td>State University of New York, Buffalo, NY 14214</td>
</tr>
<tr>
<td>Professor Steven George</td>
<td>Department of Chemistry</td>
<td>Stanford University, Stanford, CA 94305</td>
</tr>
<tr>
<td>Professor Larry Kesmodel</td>
<td>Department of Physics</td>
<td>Indiana University, Bloomington, IN 47403</td>
</tr>
<tr>
<td>Dr. Duncan Brown</td>
<td>Advanced Technology Materials</td>
<td>520-D Danury Rd., New Milford, CT 06776</td>
</tr>
<tr>
<td>Professor Tom George</td>
<td>Dept. of Chemistry and Physics</td>
<td>State University of New York, Buffalo, NY 14260</td>
</tr>
<tr>
<td>Professor Max Lagally</td>
<td>Dept. Metal. &amp; Min. Engineerir</td>
<td>University of Wisconsin, Madison, WI 53706</td>
</tr>
<tr>
<td>Professor Carolyn Cassady</td>
<td>Department of Chemistry</td>
<td>Miami University, Oxford, OH 45056</td>
</tr>
<tr>
<td>Dr. Robert Hamers</td>
<td>IBM T.J. Watson Research Center</td>
<td>P.O. Box 218, Yorktown Heights, NY 10598</td>
</tr>
<tr>
<td>Dr. Stephen Lieberman</td>
<td>Naval Ocean Systems Center</td>
<td>San Diego, CA 92152</td>
</tr>
<tr>
<td>Professor R.P.H. Chang</td>
<td>Dept. Matls. Sci. &amp; Engineering</td>
<td>Northwestern University, Evanston, IL 60208</td>
</tr>
<tr>
<td>Professor Charles Harris</td>
<td>Department of Chemistry</td>
<td>University of California, Berkeley, CA 94720</td>
</tr>
<tr>
<td>Professor M.C. Lin</td>
<td>Department of Chemistry</td>
<td>Emory University, Atlanta, GA 30322</td>
</tr>
<tr>
<td>Professor Frank DiSalvo</td>
<td>Department of Chemistry</td>
<td>Cornell University, Ithaca, NY 14853</td>
</tr>
<tr>
<td>Professor John Hemminger</td>
<td>Department of Chemistry</td>
<td>University of California, Irvine, CA 92717</td>
</tr>
<tr>
<td>Professor Fred McLafferty</td>
<td>Department of Chemistry</td>
<td>Cornell University, Ithaca, NY 14853-1301</td>
</tr>
<tr>
<td>Dr. James Duncan</td>
<td>Federal Systems Division</td>
<td>Eastman Kodak Company, Rochester, NY 14650-2156</td>
</tr>
<tr>
<td>Professor Leonard Interrante</td>
<td>Department of Chemistry</td>
<td>Rensselaer Polytechnic Institute, Troy, NY 12181</td>
</tr>
<tr>
<td>Professor Horia Metiu</td>
<td>Department of Chemistry</td>
<td>University of California, Santa Barbara, CA 93106</td>
</tr>
<tr>
<td>Professor Arthur Ellis</td>
<td>Department of Chemistry</td>
<td>University of Wisconsin, Madison, WI 53706</td>
</tr>
<tr>
<td>Professor Roald Hoffmann</td>
<td>Department of Chemistry</td>
<td>Cornell University, Ithaca, NY 14853</td>
</tr>
<tr>
<td>Professor Larry Miller</td>
<td>Department of Chemistry</td>
<td>University of Minnesota, Minneapolis, MN 55455-0431</td>
</tr>
<tr>
<td>Professor Mustafa El-Sayed</td>
<td>Department of Chemistry</td>
<td>University of California, Los Angeles, CA 90024</td>
</tr>
<tr>
<td>Professor Eugene Irene</td>
<td>Department of Chemistry</td>
<td>University of North Carolina, Chapel Hill, NC 27514</td>
</tr>
<tr>
<td>Professor George Morrison</td>
<td>Department of Chemistry</td>
<td>Cornell University, Ithaca, NY 14853</td>
</tr>
</tbody>
</table>