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Change in Density of States in a Resonant Tunneling Structure due to a Scattering Center in the Well

by

L. N. Pandey, Thomas F. George, M. L. Rustgi and D. Sahu

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Change in density of states in a resonant tunneling structure due to a scattering center in the well

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

M. L. Rustgi
Department of Physics & Astronomy
State University of New York at Buffalo
Buffalo, New York, 14260

and

D. Sahu
Computer Sciences Corporation
10110 Aerospace Road
Lanham-Seabrook, Maryland 20706

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INTRODUCTION

The progress of semiconductor fabrication technology, particularly the molecular beam epitaxy (MBE), has permitted the construction of structures and devices whose properties are dominated by quantum interference effects. Recently, very narrow potential barrier profiles have been produced in $GaAs$ / $Al_xGa_{1-x}As$ superlattices.[1,2] The intentional doping has been implemented by positioning Si donors and Be acceptors in precise numbers during the MBE growth of $GaAs$ layers. This so-called sheet-doping (or delta-doping) technique, originally proposed by Wood et al,[3] has been applied in advanced semiconductor device techniques. The confinement of donors or acceptors to selectively doped $GaAs$ /$Al_xGa_{1-x}As$ heterostructures leads to high mobilities and to high two-dimensional carrier densities. Since the early studies by Chang,Tsu and Esaki[4-6] of resonant tunneling through quantum-well states and negative differential resistance in double barriers heterostructures, there have been numerous investigations of one-dimensional resonant tunneling structures (RTS) and quantum wells (QW). These RTS and QW are not only important in microdevices but their study involves a great deal of basic physics. Most of the theoretical investigations of the static properties of the RTS have been limited to the calculation of transmission coefficients through the interfaces of the RTS. However, in recent years it has been realized that the study of the electronic density of states of RTS is equally important due to the applicability of RTS and QW in optical devices.[7] It has also been noticed that the density of states provide a better representation of states in comparison with the transmission coefficients

since there are some circumstances where transmission coefficients do not exist.

There have been different approaches to study the electronic density of states of RTS. For example, Bahdr and coworkers[3] calculated the local density of states by means of Green's functions. Their calculations were for the RTS where the two barriers are represented by two delta(δ)-function potentials, and later they included the finite width for the barriers in their calculations. The global density of states from the local density of states of Ref. 8 can be shown to be identically zero. Bloss[9] has calculated the wave function in the well region of the RTS under bias. He has shown that the integral value of the square of the wave function over the well region of the RTS and the density of states are correlated. Kim and Arnold[10] have also performed some calculations for the local density of states using the nonequilibrium tunneling theory of Caroli et al[11] and the scattering-theoretic Green's-function technique with a simple Hamiltonian. However, none of these investigations have considered the effect of a scattering center on the density of states.

A model calculation of the electronic states of a superlattice of period a interleaved with a periodic array of δ-function impurity centers has been reported by Beltram and Capasso[12], who found that through a judicious choice of the width of the quantum well and location of the impurity, the width of the minibands could be controlled. Earlier, Stone and Lee [13] had considered the effect of inelastic scattering on tunneling resonances in one dimension.

Recently, we presented a simple technique to calculate the change in the global density of states of RTS.[14,15] The technique described in Refs. 14 and

15 is suitable for calculating the global density of states for any potential profile within a box. This density was calculated for the RTS in the box and compared with the density of states of the empty box. We found that the states are piled up at the resonance energies and pushed away in the energy regions away from the resonance energies. A plot of the density of states versus energy shows a peak at the transmission resonance energies if the resonance is sharp. Otherwise the peak of this plot is shifted from the transmission resonance energy. A linear decrease in the resonance energy and broadening of the states as a function of bias voltage are observed.[15] For an asymmetric RTS, the plots of transmission coefficients and the change in density of states have left-right symmetry with respect to the interchange of the two barriers of the RTS. This symmetry is broken in the case of an asymmetric RTS under bias.

In this paper, we have used an extra thin barrier or a δ-function potential in the well to describe the perturbation potential of a scattering center and study its effect on the transmission and change in the global density of states. The corresponding changes in the bound states of the RTS are important in the interstate transition studies. It is found that the extra thin barrier and δ-function potential in the middle of the well moves the even bound states up, while the odd states remains unchanged. The widths of the even states get broader as the thin barrier height increases or the strength of the δ-function potential increases. The density of states for the energies of even states is reduced due to the broadening of the states.

CALCULATIONAL TECHNIQUE

The method to calculate the transmission coefficients T(E) as function of electron energy E through a potential profile such as RTS are well described in the literatures.[16,17] To calculated the global density of states, the procedure laid out in Refs. 14 and 15 is followed here. For the sake of completeness, a brief description to calculate the density of states is given below. The local density of states is

$$N(E,x) = \sum_j \delta(E - E_j)|\Psi(x,E_j)|^2, \tag{1}$$

where $\Psi(x,E_j)$ and E_j are the eigenfunctions and eigenvalues, respectively. The global density of states obtained by integrating Eq. (1) will be identically zero.[8] Therefore, a different method to calculate the global density of states,

$$N(E) = \sum_j \delta(E - E_j),$$

has been adopted here. In this way, a change in the spacing of energy levels brought in by RTS contributes to the density of states without involving any particular spatial region. Let us consider a box of length L and walls extended to infinity. The eigenstates of this box, $\frac{n\pi}{L}$ where n is an integer, are equally spaced in k-space, and the inverse of the spacing, which is the density of states, is constant for a given L and increases linearly with L. The spacing of eigenstates becomes disturbed by a small RTS in the box. This change in the spacing brought by the RTS has been calculated to find the change in the global density of states. The RTS in the box produces a phase change in the eigenfunction. The solution of the Schrödinger equation for an electron in a box extending from

0 to L is $\sqrt{\frac{2}{L}}\sin(\frac{n\pi}{L}x)$, and the solution for an electron in a box with the RTS is $A\sin(\frac{n\pi}{L}+\phi)x$ with A as a normalization constant. Depending upon the the position of the RTS in the box, the phase difference, ϕ, forms different patterns, where each pattern is called a subdensity.[14] The sum of changes contributed by all the subdensities gives the change in the global density of states due to the RTS.

A schematic illustration of the structure considered here is given in Fig. 1. An RTS of a few hundred Å total width with an extra thin barrier or a δ-function potential in the well region is placed in a box of length L. The value of L ranges from 10^6 to 10^8 Å depending upon the resolution needed for resonance states. The RTS is placed at a distance x_1 from the left wall of the box. The two barriers of the RTS extend from x_1 to x_1+a_1 and x_1+a_1+d to $x_1+a_1+d+a_2$, where d is the well width and a_1 and a_2 are widths of the left and right barriers. The heights of the barriers are V_L and V_R. A thin barrier of variable height and fixed width, b, ranging from $x_1+a_1+\frac{d-b}{2}$ to $x_1+a_1+\frac{d+b}{2}$ where b$\ll$d, or a δ-function potential at $x_1+a_1+c(\leq x_1+a_1+d)$, in the well has been considered as an extra potential profile in the RTS. The eigenvalue condition, namely the vanishing of the wave function at x=L, can be given as

$$D(k) = A_4(k)\sin k(L-x_2) + B_4(k)\cos k(L-x_2) = 0, \qquad (2)$$

where $x_2 = x_1+a_1+d+a_2$ and $A_4(k)$ and $B_4(k)$ are the amplitudes of the envelop wave function in the region from $x = x_2$ to x=L. The amplitudes $A_4(k)$ and $B_4(k)$ can be calculated easily by requiring wave functions and their derivatives to be continuous across the interfaces of the RTS. Here $k = \sqrt{\frac{2m^*E}{\hbar^2}}$ and m^* is the

effective mass of the electron. A constant value of m^* (=0.067m_e, with m_e as the electron mass) has been taken throughout the structure in our calculation for simplicity. For the case of a different effective mass, the derivative of the wave function divided by the effective mass of the region should be continuous instead of the derivative alone.[18-20] The positions of the resonance states get lowered slightly, but the widths of the states broaden considerably for the case in which one considers different effective masses.[21] So, in the calculation where a comparison with the experiment, especially the dwell time, is undertaken, the correct value of the effective masses of different materials should be considered.

The change in the density of states in k-space in comparison with a free box can be calculated as

$$\Delta N(k_n) = \frac{1}{\Delta k_n} - \frac{L}{n\pi}, \tag{3a}$$

and hence,

$$\Delta N(E) = \Delta N(k)\frac{m^*}{\hbar^2 k}. \tag{3b}$$

Here $\Delta k_n = k_n - k_{n-1}$ and k_n and k_{n-1} are calculated from Eqn. (2). As mentioned earlier, ΔN(k) or ΔN(E) should be calculated for all the subdensities and summed over all subdensities to give the change in global density of states.

RESULTS AND DISCUSSION

The structure under investigation is shown in Fig. 1 for an asymmetric RTS in a box. Parameters used in the calculation are as follows: for a symmetric RTS, $a_1 = a_2$= 50 Å, d=150 Å and $V_L = V_R$=200 meV, and for an asymmetric RTS, $a_1 = a_2$= 50 Å, d=150 Å, V_L=200 meV and V_R=180 meV. The position of the symmetric and asymmetric RTS is $x_1 = \frac{L}{2}$, at which two subdensities are formed.

For the parameters described above, there are three resonances at 16.5± 0.0434, 64.87± 0.540 and 140.76± 3.72 meV for the symmetric RTS, and 16.33± 0.0533, 64.1± 0.661 and 138.8± 4.49 meV for the asymmetric one. The escape times for these three resonance states, $t_{es} = \frac{\hbar}{\delta E}$, where δE is the width of the states, are 15.2, 1.22 and 0.177 ps for the symmetric RTS, and 12.3, 1.0 and 0.147 ps for the asymmetric one, respectively. It is clear that as the states move closer to the surface of the well, the escape times get smaller and smaller. An electron at the state deep inside the well takes more time to tunnel through the barriers than the one at the state closer to the surface of the well, which is a signature of the time-energy uncertainty relation.

On the left side of the Fig. 2, the results for transmission T(E) and change in density of states, ΔN(E) for the symmetric (solid curves) and for the asymmetric RTS (dashed curves) with a thin barrier of 15 Å width and 10 meV height as an extra potential profile are shown in the first resonance energy range. For the sake of comparison, results without an extra potential profile (dotted for symmetric and dot-dashed for asymmetric RTS) are also plotted in Fig. 2. Corresponding results for a δ-function potential (100 meV·Å strength in the middle of the well) as an extra potential profile are displayed on the right side of the Fig. 2. It is clear that the energy of the first resonance state shifts towards the higher energy for both the thin barrier and δ-function potentials. As mentioned earlier, the width of the state which shifts towards the surface of the well should increase from the time-energy uncertainity relation. This behavior is not quite apparent from the Fig. 2 because of the narrowness of the state. The peak value of

ΔN(E) is reduced in comparison with the peak value of ΔN(E) for the RTS without an extra potential profile. However, T(E) attains the value of unity for the symmetric RTS and reduces to a definite value less than unity for the asymmetric one. The reason for the change in ΔN(E) is that a quantity

$$\Delta N = \int dE \Delta N(E) \tag{4}$$

should have the value of unity for a single bound state. For ΔN to be unity, a lower value of ΔN(E) at the resonance energy makes it clearer that the width of the resonance has increased for a finite value of the thin barrier height and finite strength of the δ-function potential. A further discussion of the quantity ΔN is given later in the text. Although there is no direct correlation between the width and height of the thin barrier and the strength of the δ-function potential, a correspondence between them can be derived from Fig. 2.

The results for the second resonance state are shown in Fig. 3. In this figure the change in resonance energy due to the thin barrier is very small, and there is no change at all for the δ-function potential. The reason for such behavior can be attributed to the nature of the wave function of the second resonance state. A normalized wave function of the first, second and third resonance states with a thin barrier height and width of 65 meV and 15 Å, respectively (upper panel), and with a δ-function potential of strength of one eV·Å (lower panel) as an extra potential profile to the RTS, are shown in Fig. 4. As expected, the wave function of the second resonance state vanishes in the middle of the well, and an extra potential profile present in the middle of the well remains unseen by it. Due to the finite width of the thin barrier, the envelop wave function

gets affected over a spatial range, where the small change in resonance energy is a result of such effect. Moreover, the δ-function potential is confined to a particular position in spatial dimension and affects only the derivatives of the wave function. If the position of the δ-function potential is at a point (middle of the well) where the wave function of the second resonance state vanishes, then its effect will be absolutely zero on the second resonance state. The results for the third resonance are similar to those of the first resonance due to the similarity in their wave functions, and are not shown here for brevity.

The change in resonance energy and width of the resonance state and the change in density of states $\Delta N(E)$ at the resonance energy for the first and second resonance states as a function of thin barrier height (15 Å width) and as a function of the strength of the δ-function potential at c=0 are shown in Figs. 5 and 6. In Fig. 5, the change in energy of the first resonance state for the symmetric and asymmetric RTS are indistinguishable. Moreover, the increase in the width of the resonance is more pronounced for the asymmetric RTS than the symmetric one. It is clear from earlier discussions (about the width and escape time) that the escape time from a state is less for an asymmetric RTS than from the corresponding state of a symmetric RTS. As we mentioned earlier, the peak value of $\Delta N(E)$ decreases for a finite height of the thin barrier and finite strength of the δ-function potential. This decrease in $\Delta N(E)$ is correlated with the increase in widths of the resonance states through the quantity ΔN [Eq. (4)], but the variation of the width as a function of thin barrier height and strength of the δ-function potential in Fig. 5 is entirely different than the

variation of $\Delta N(E)$. The tails of the Gaussian distribution persist longer for the broader distribution and contribute more to the area of the distribution. Hence, the increase in the width does bring the peak value of $\Delta N(E)$ down, but the condition $\Delta N=1$ makes it decrease faster than the increase in the width. The energy of the first resonance state increases exponentially as a function of the thin barrier height and the strength of the δ-function potential and approaches the second resonance state. In Fig. 6, as discussed earlier, changes brought about by the thin barrier and δ-function potential are negligible. So, the extra potential profile could cause the first resonance state to merge into the second resonance state. The changes in the third resonance state are similar to those in the first one.

CONCLUSIONS

In conclusion, we have studied the effect of a scattering center on the transmission and change in density of states for both symmetric and asymmetric resonant tunneling structures by representing it by a thin barrier of variable height and fixed width, and by a δ-function potential of variable strength, and placing it in the middle of the well. It is found that because of the extra profile the resonance energies are shifted up, and the widths of the resonance states are increased for the even states. The change in width is the signature of the time-energy uncertainity relation. There are practically no changes in the odd states because of the nature of their wave functions. The peak value of a plot of the change in density of states versus the energy decreases as the height of the thin barrier or the strength of the δ-function potential increases. This decrease

is related to the change in the width of the resonance states.

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FIGURE CAPTIONS

Fig. 1. Schematic illustration of an asymmetric RTS structure with an extra potential profile in a box. The position of the RTS in the box is x_1 from the left wall. The widths and heights of the two barriers of the RTS are, respectively, a_1 & a_2 and V_L & V_R, and the well width is d. A thin barrier of width b and variable height and a δ-function potential as shown are considered as an extra potential profile in the RTS.

Fig. 2. Transmission coefficient T(E) and change in density of states ΔN(E) for a symmetric (solid curve) and asymmetric (dashed curved) RTS with a thin barrier of 15 Å width and 10 meV height and δ-function potential of 100 meV·Å strength, compared with T(E) and ΔN(E) for a symmetric (dotted curve) and asymmetric (dot-dashed curve) RTS with zero thin barrier height and zero δ-function potential strength. The energy range shown is in the neighborhood of the first resonance state.

Fig. 3. T(E) and ΔN(E) for the second resonance state. The different curves are described in Fig. 2.

Fig. 4. Wave functions of the first (solid curve),second (dashed curve) and third (dotted curve) resonance states for a thin barrier of height 65 meV and width 15 Å(top panel) and a δ-function potential of strength one eV·Å (bottom panel).

Fig. 5. Change in resonance energy, width of the resonance state and peak value of the ΔN(E) versus E plot of the first resonance state for the symmetric (solid circles) and asymmetric (solid triangle) RTS as a

function of thin barrier height (15 Å width) and the strength of δ-function potential.

Fig. 6. Same as in Fig. 5 but for the second resonance state.

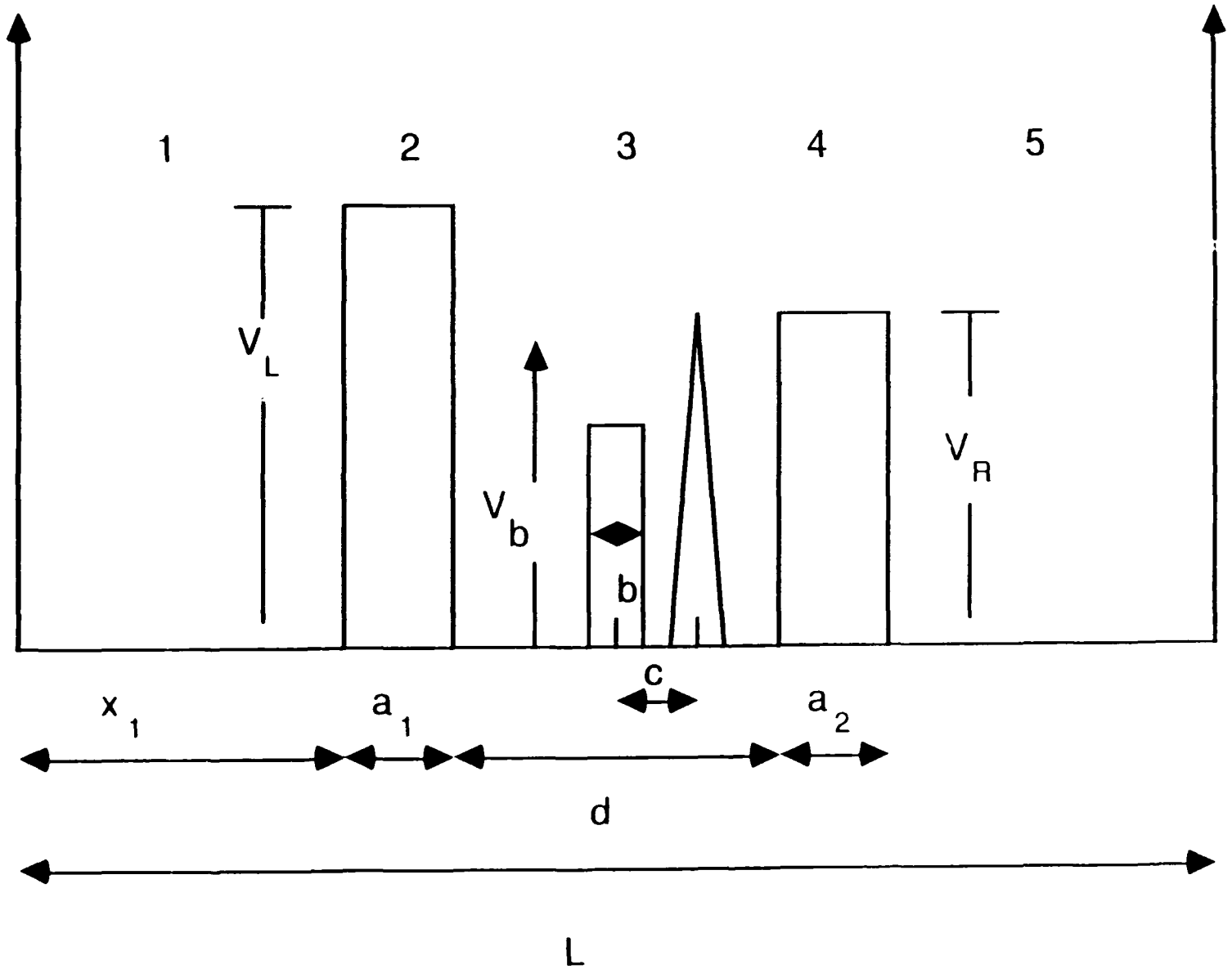

1
2
3
4
5
V_L
V_b
b
V_R
c
x_1
a_1
a_2
d
L

Fig 2

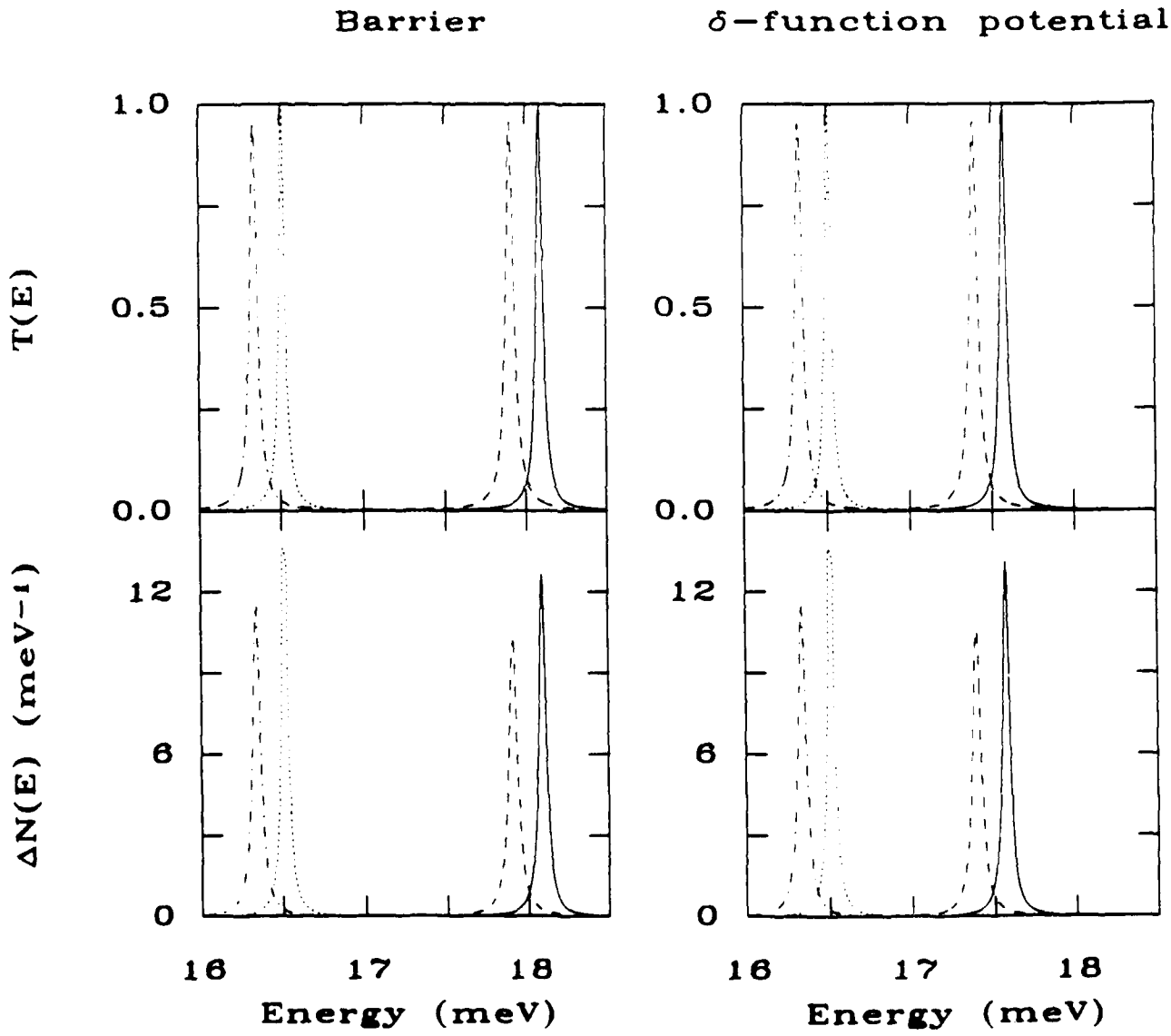
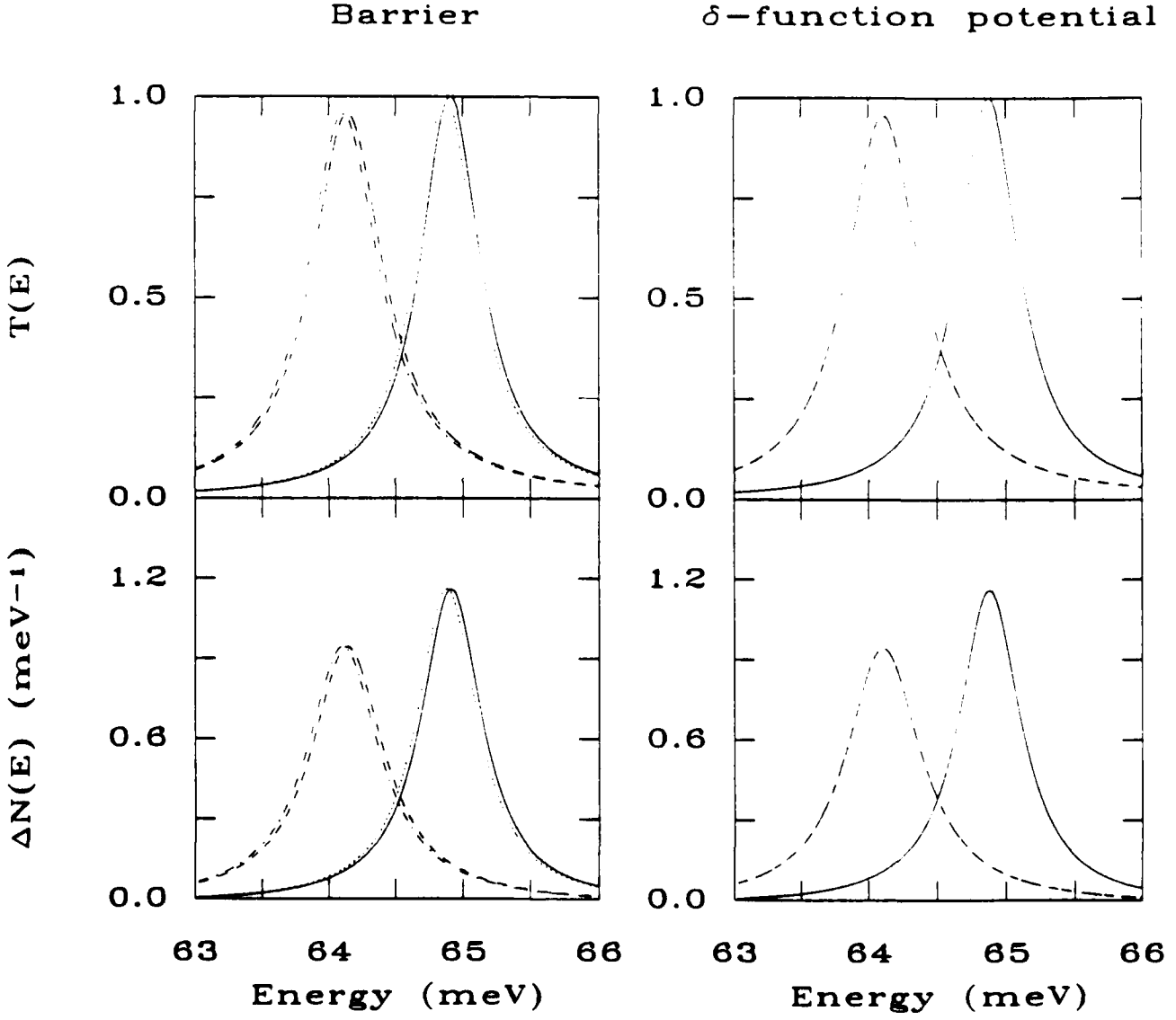

Barrier
δ−function potential
T(E)
ΔN(E) (meV⁻¹)
1.0
0.5
0.0
12
6
0
16
17
18
Energy (meV)

Fig 3


Barrier
δ−function potential
T(E)
ΔN(E) (meV⁻¹)
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0.5
0.0
1.2
0.6
0.0
63
64
65
66
Energy (meV)

Fig 4

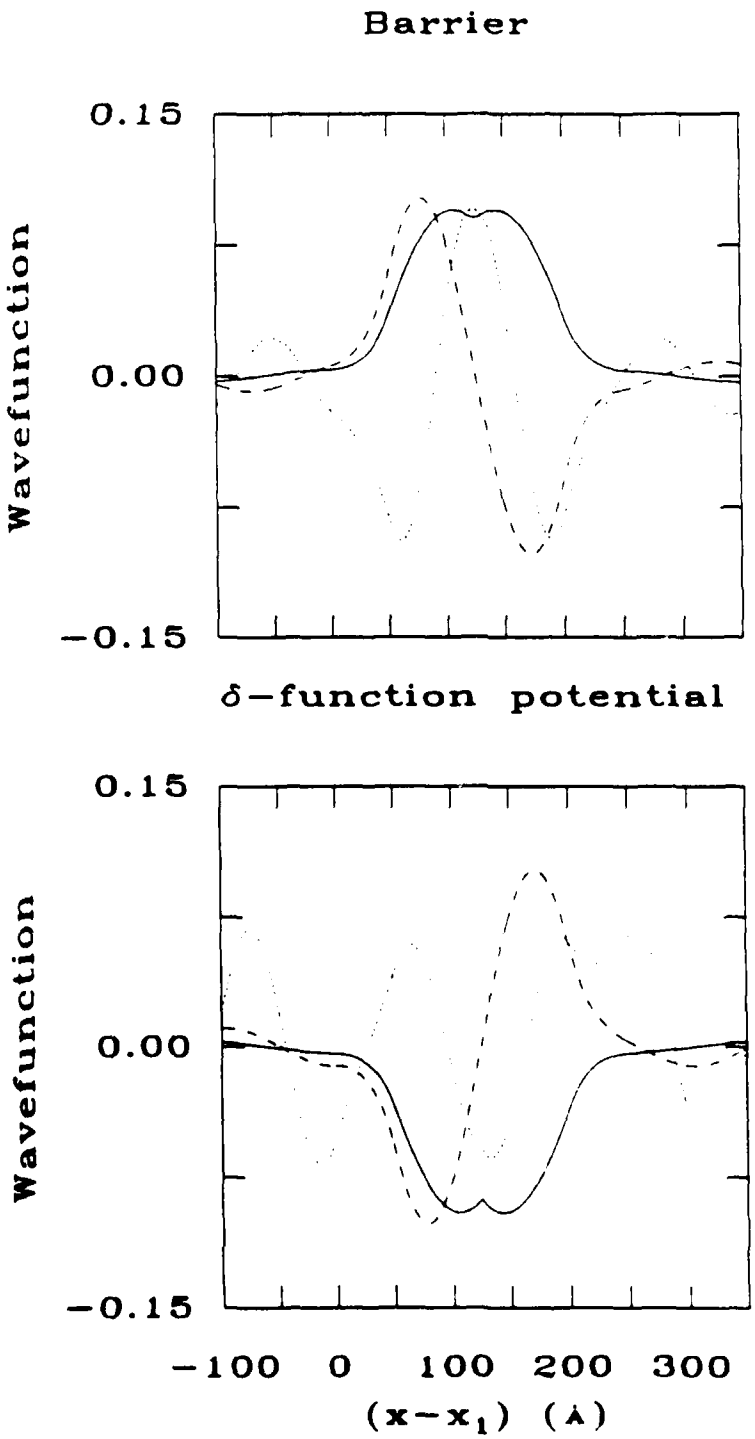

Barrier
0.15
0.00
−0.15
Wavefunction
δ−function potential
0.15
0.00
−0.15
Wavefunction
−100
0
100
200
300
(x−x1) (Å)

Fig 5

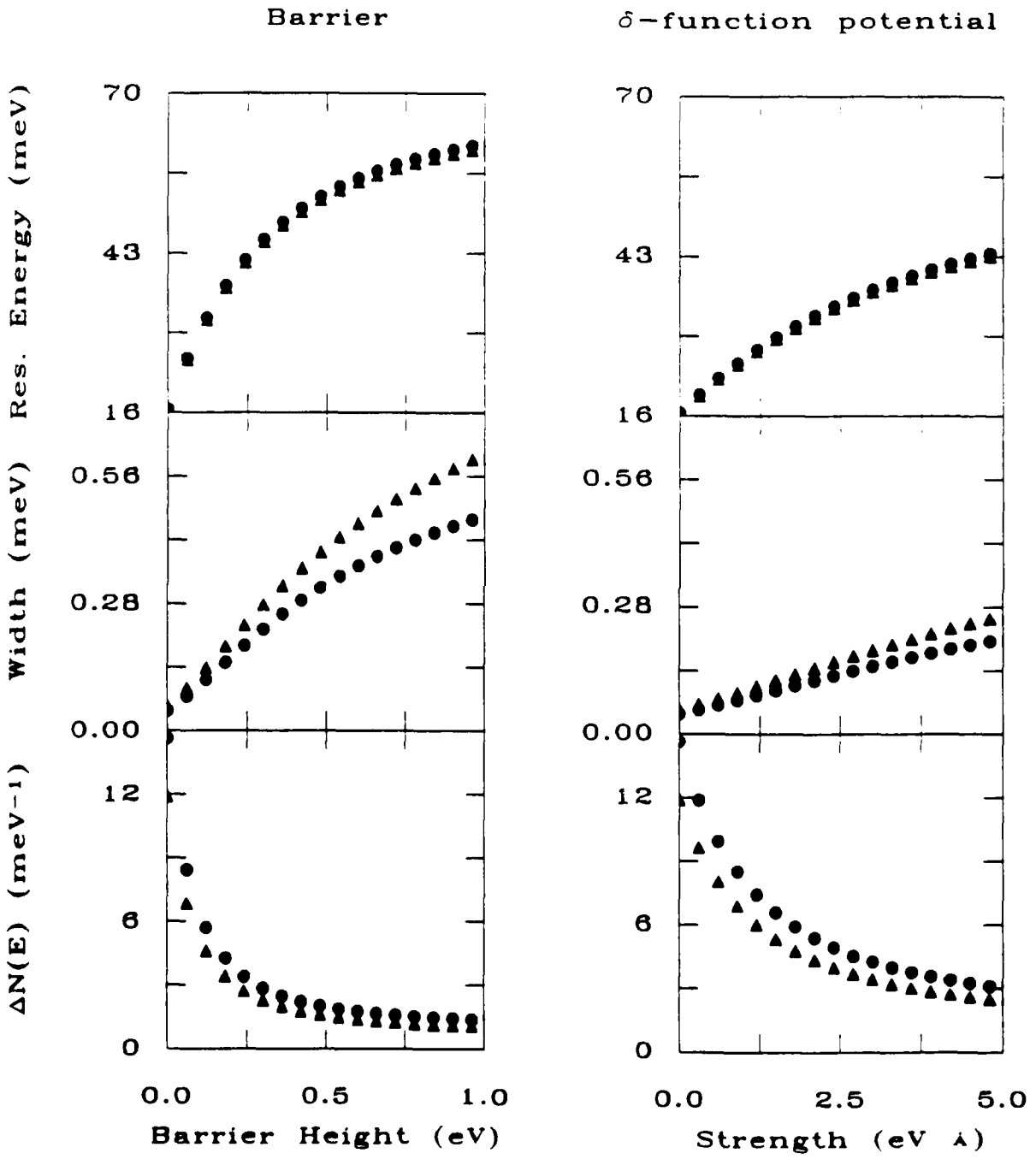
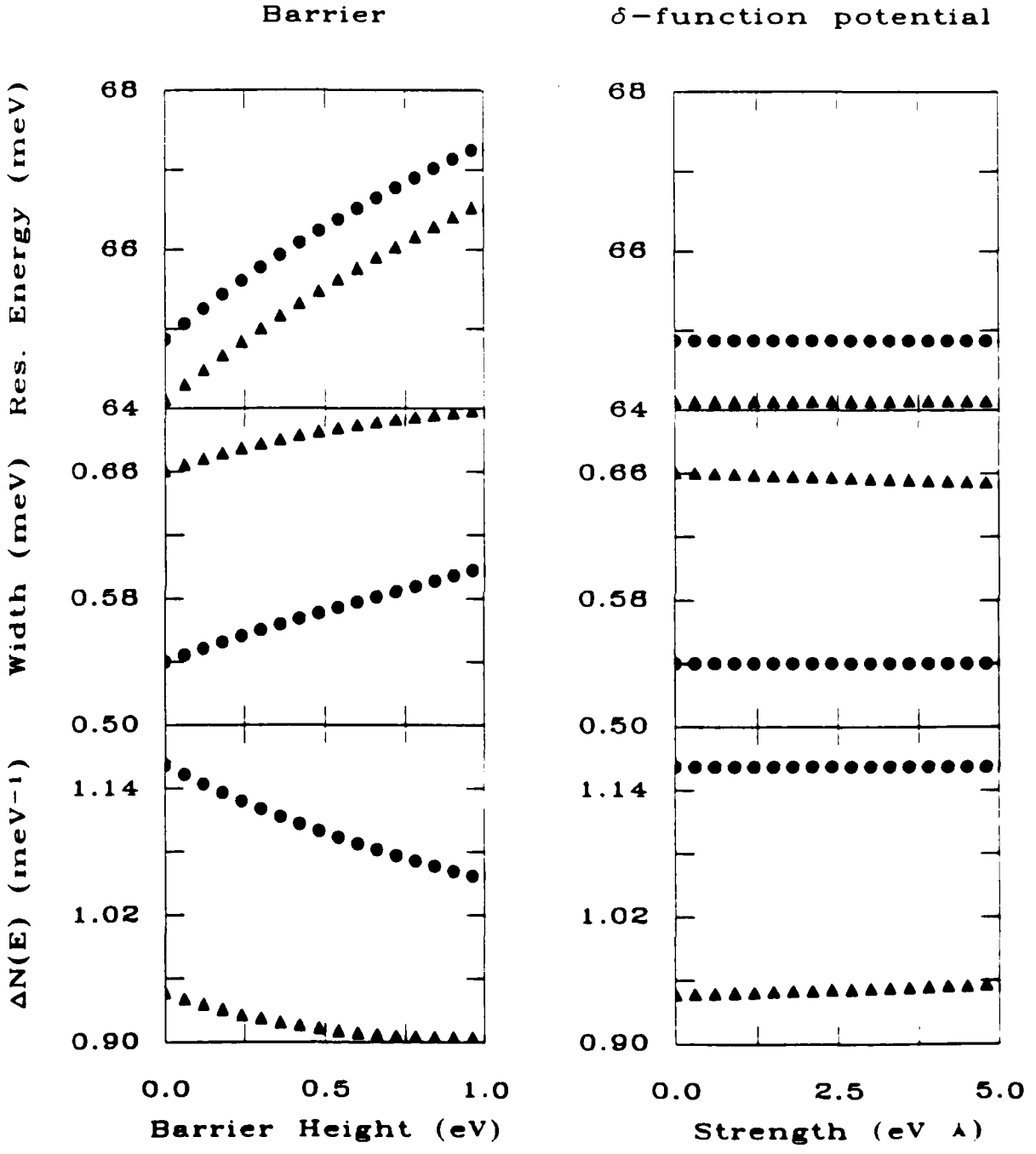

Barrier
δ-function potential
Res. Energy (meV)
Width (meV)
ΔN(E) (meV⁻¹)
70
43
16
0.56
0.28
0.00
12
6
0
0.0
0.5
1.0
Barrier Height (eV)
0.0
2.5
5.0
Strength (eV Å)

Fig 6


Barrier
δ−function potential
Res. Energy (meV)
Width (meV)
ΔN(E) (meV⁻¹)
68
66
64
0.66
0.58
0.50
1.14
1.02
0.90
0.0
0.5
1.0
2.5
5.0
Barrier Height (eV)
Strength (eV Å)

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Dr. Richard W. Drisko (1)
Naval Civil Engineering Laboratory
Code L52
Port Hueneme, CA 93043

David Taylor Research Center (1)
Dr. Eugene C. Fischer
Annapolis, MD 21402-5067

Dr. James S. Murday (1)
Chemistry Division, Code 6100
Naval Research Laboratory
Washington, D.C. 20375-5000

Dr. David L. Nelson (1)
Chemistry Division
Office of Naval Research
800 North Quincy Street
Arlington, Virginia 22217

Dr. Robert Green, Director (1)
Chemistry Division, Code 385
Naval Weapons Center
China Lake, CA 93555-6001

Chief of Naval Research (1)
Special Assistant for Marine Corps Matters
Code 00MC
800 North Quincy Street
Arlington, VA 22217-5000

Dr. Bernadette Eichinger (1)
Naval Ship Systems Engineering Station
Code 053
Philadelphia Naval Base
Philadelphia, PA 19112

Dr. Sachio Yamamoto (1)
Naval Ocean Systems Center
Code 52
San Diego, CA 92152-5000

Dr. Harold H. Singerman (1)
David Taylor Research Center
Code 283
Annapolis, MD 21402-5067

Defense Technical Information Center (2)
Building 5, Cameron Station
Alexandria, VA 22314

FY90 Abstracts Distribution List for Solid State & Surface Chemistry

Professor John Baldeschwieler
Department of Chemistry
California Inst. of Technology
Pasadena, CA 91125

Professor Paul Barbara
Department of Chemistry
University of Minnesota
Minneapolis, MN 55455-0431

Dr. Duncan Brown
Advanced Technology Materials
520-B Danury Rd.
New Milford, CT 06776

Professor Stanley Bruckenstein
Department of Chemistry
State University of New York
Buffalo, NY 14214

Professor Carolyn Cassady
Department of Chemistry
Miami University
Oxford, OH 45056

Professor R.P.H. Chang
Dept. Matls. Sci. & Engineering
Northwestern University
Evanston, IL 60208

Professor Frank DiSalvo
Department of Chemistry
Cornell University
Ithaca, NY 14853

Dr. James Duncan
Federal Systems Division
Eastman Kodak Company
Rochester, NY 14650-2156

Professor Arthur Ellis
Department of Chemistry
University of Wisconsin
Madison, WI 53706

Professor Mustafa El-Sayed
Department of Chemistry
University of California
Los Angeles, CA 90024

Professor John Eyler
Department of Chemistry
University of Florida
Gainesville, FL 32611

Professor James Garvey
Department of Chemistry
State University of New York
Buffalo, NY 14214

Professor Steven George
Department of Chemistry
Stanford University
Stanford, CA 94305

Professor Tom George
Dept. of Chemistry & Physics
State University of New York
Buffalo, NY 14260

Dr. Robert Hamers
IBM T.J. Watson Research Center
P.O. Box 218
Yorktown Heights, NY 10598

Professor Paul Hansma
Department of Physics
University of California
Santa Barbara, CA 93106

Professor Charles Harris
Department of Chemistry
University of California
Berkeley, CA 94720

Professor John Hemminger
Department of Chemistry
University of California
Irvine, CA 92717

Professor Roald Hoffmann
Department of Chemistry
Cornell University
Ithaca, NY 14853

Professor Leonard Interrante
Department of Chemistry
Rensselaer Polytechnic Institute
Troy, NY 12181

Professor Eugene Irene
Department of Chemistry
University of North Carolina
Chapel Hill, NC 27514

Dr. Sylvia Johnson
SRI International
333 Ravenswood Avenue
Menlo Park, CA 94025

Dr. Zakya Kafafi
Code 6551
Naval Research Laboratory
Washington, DC 20375-5000

Professor Larry Kesmodel
Department of Physics
Indiana University
Bloomington, IN 47403

Professor Max Lagally
Dept. Metal. & Min. Engineering
University of Wisconsin
Madison, WI 53706

Dr. Stephen Lieberman
Code 522
Naval Ocean Systems Center
San Diego, CA 92152

Professor M.C. Lin
Department of Chemistry
Emory University
Atlanta, GA 30322

Professor Fred McLafferty
Department of Chemistry
Cornell University
Ithaca, NY 14853-1301

Professor Horia Metiu
Department of Chemistry
University of California
Santa Barbara, CA 93106

Professor Larry Miller
Department of Chemistry
University of Minnesota
Minneapolis, MN 55455-0431

Professor George Morrison
Department of Chemistry
Cornell University
Ithaca, NY 14853

Professor Daniel Neumark
Department of Chemistry
University of California
Berkeley, CA 94720

Professor David Ramaker
Department of Chemistry
George Washington University
Washington, DC 20052

Dr. Gary Rubloff
IBM T.J. Watson Research Center
P.O. Box 218
Yorktown Heights, NY 10598

Professor Richard Smalley
Department of Chemistry
Rice University
P.O. Box 1892
Houston, TX 77251

Professor Gerald Stringfellow
Dept. of Matls. Sci. & Engineering
University of Utah
Salt Lake City, UT 84112

Professor Galen Stucky
Department of Chemistry
University of California
Santa Barbara, CA 93106

Professor H. Tachikawa
Department of Chemistry
Jackson State University
Jackson, MI 39217-0510

Professor William Unertl
Lab. for Surface Sci. & Technology
University of Maine
Orono, ME 04469

Dr. Terrell Vanderah
Code 3854
Naval Weapons Center
China Lake, CA 93555

Professor John Weaver
Dept. of Chem. & Mat. Sciences
University of Minnesota
Minneapolis, MN 55455

Professor Brad Weiner
Department of Chemistry
University of Puerto Rico
Rio Piedras, Puerto Rico 00931

Professor Robert Whetten
Department of Chemistry
University of California
Los Angeles, CA 90024

Professor R. Stanley Williams
Department of Chemistry
University of California
Los Angeles, CA 90024

Professor Nicholas Winograd
Department of Chemistry
Pennsylvania State University
University Park, PA 16802

Professor Aaron Wold
Department of Chemistry
Brown University
Providence, RI 02912

Professor Vicki Wysocki
Department of Chemistry
Virginia Commonwealth University
Richmond, VA 23284-2006

Professor John Yates
Department of Chemistry
University of Pittsburgh
Pittsburgh, PA 15260