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A THEORY OF EXCITON PHOTOLUMINESCENCE FOR TWO TYPES OF NEUTRAL ACCEPTORS IN SILICON -A STUDY OF THE SYSTEMS Si:(B,In), Si:(Al,In), Si:(Ga,In), Si:(B,Al), Si:(B,Ga), and Si:(Al,Ga)

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FEBRUARY 1985

INTERIM REPORT FOR PERIOD JUNE 1983 - AUGUST 1984

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G. EDWARD KUHL, Chief

Laser & Optical Materials Branch

Electromagnetic Materials Division

This technical report has been reviewed and is approved for publication.

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DAVID W. FISCHER Project Monitor Laser & Optical Materials Branch

FOR THE COMMANDER

NERRILL L. MINGES, Chief Electromagnetic Materials Division Materials Laboratory Air Force Wright Aeronautical Laboratories

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19. Abstract (Continued)

with large differences in the bound exciton energy levels such as Si:(B,In), Si:(Al,In), and Si:(Ga,In), and having indium concentrations exceeding 10^{15} cm⁻³, it predicts quenching of shallow impurity bound exciton luminescence, because the forward exciton tunneling rate from the shallow level to the deep level of indium dominates and the reverse exciton tunneling rate from indium to the shallow impurities is negligible. For the systems with small differences in the bound exciton energy levels such as Si:(B,Al) and Si:(B,Ga), the theory predicts enhancement of shallow impurity bound exciton luminescence beyond certain concentrations depending upon the free exciton capture cross section ratios because in these cases the reverse exciton tunneling rate dominates. For the system Si:(Al,Ga) in which the difference in the bound exciton energy levels is very small, gallium bound exciton luminescence dominates when the gallium concentration exceeds 10^{16} cm⁻³ if the aluminum free exciton capture cross section is less than the gallium free exciton capture cross section. The energy eigenvalue equation for an exciton in a one-dimensional finite double potential well is derived for future use.

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SUMMARY

Rate equations for the densities of free excitons and excitons bound to two types of neutral acceptors in silicon are solved for steady state in the absence of saturation. These rate equations explicitly include the terms for reverse and forward tunneling of bound excitons from one type of neutral impurity to another. The tunneling rates are calculated using a simple model of an exciton in a one-dimensional semi-infinite double potential well. The energy eigenvalue equation for an exciton in this potential well is derived for estimating the exciton tunneling time. The steady-state solutions of the rate equations yield an expression for the ratio of the bound exciton luminescence intensity as a function of the impurity concentrations. The relative photoluminescence intensities for the systems Si: (B,In), Si: (Al,In), Si: (Ga,In), Si: (B,Al), Si: (B,Ga), and Si(Al,Ga) are calculated for various values of the relevant free exciton capture cross section ratios. This model predicts no exciton tunneling for any of the above systems for the low impurity concentration range of $10^{12}-10^{14}$ cm⁻³. For the systems with large differences in the bound exciton energy levels such as Si: (B,In), Si: (Al,In), and Si: (Ga,In), and having indium concentrations exceeding 10^{15} cm³, it predicts guenching of shallow impurity bound exciton luminescence because the forward exciton tunneling rate from the shallow level to the deep level of indium dominates and the reverse exciton tunneling rate from indium to the shallow impurities is negligible. For the systems with small differences in the bound exciton energy levels such as Si:(B,Al) and Si: (B,Ga), the theory predicts enhancement of shallow impurity

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FOREWORD

Materials requirements for silicon-based devices are becoming ever more stringent as VHSIC-related applications become more important to Air Force research. Photoluminescence (PL) has been shown to be an effective method for impurity and defect concentration determination in the $10^{11}-10^{13}$ cm⁻³ range. However, recent experimental and theoretical evidence indicates that the PL method may have limited usefulness as a quantitative technique for impurity concentrations above 10^{15} cm⁻³. This paper establishes a theoretical framework for examining the exciton tunneling problem in doubly-doped silicon and thus establishes a "window of applicability" for quantitative concentration measurements in silicon.

One of the authors (D. S. Moroi) would like to thank the AFOSR for supporting the preliminary part of the work under the 1982 USAF-SCEEE Summer Faculty Research Program, Contract No. F49620-82-C-0035 and Universal Energy Systems for funding the project for the summer months of 1983 under Contract No. F33615-82-C-5001 and Task No. 729-074. He would like to extend his appreciation to the Laser and Optical Materials Branch, Electromagnetic Materials Division, the Materials Laboratory of the AFWAL for providing him with the opportunity to spend the very worthwhile and rewarding summers. It is our pleasure to thank Dr. Patrick M. Hemenger for providing useful references and inspiring discussions. His collaboration, guidance, and continuing encouragement during the course of research is appreciated. We are also thankful to Dr. Frank Szmulowicz for

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numerous stimulating discussions on modelling exciton tunneling. Finally, we want to thank Mr. David O'Quinn for his fine work in producing many of the figures for the tunneling factors and Ms. Niki Maxwell for a fine job of typing the manuscript. TABLE OF CONTENTS

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SECTION I INTRODUCTION

Characterization of semiconductor materials in terms of their electromagnetic properties is important to the development of semiconductor devices and various electrical and optical techniques¹ have been utilized to study those electromagnetic properties. Particularly, recent progress in the technology of integrated circuits demands near-perfect crystals of silicon and requires, therefore, a great improvement in the methods of analysis for minute amounts of impurities and defects in silicon since they drastically change its electromagnetic properties.

Recently, attempts have been made to use photoluminescence (PL) as a quantitative tool for measuring impurity concentrations. Tajima² obtained boron and phosphorus concentrations in silicon crystals by PL analysis at liquid-helium temperature. Nakayama et al.³ measured and analyzed the low temperature exciton luminescence of silicon on the basis of rate equations describing the formation and decay kinetics of free excitons (FE), bound excitons (BE) and bound multiexciton complexes. Tajima and Nomura⁴ applied the PL technique to the quantitative analysis of shallow impurities incorporated intentionally and unintentionally in silicon epitaxial layers. Mitchard and McGill⁵ used PL to determine relative concentrations in the Si:(B,In) system while Brown et al.⁶ investigated the optical and electrical properties of the systems Si: (In, Al) using PL, Hall effect transport, infrared absorption, and photoconductivity measurements. In both papers, it was observed that the luminescence from the shallower acceptor (B or Al) of a two-acceptor system may be guenched when

the concentration of the deeper acceptor (In) exceeds certain critical values $(>10^{16} \text{ cm}^{-3})$.⁵⁻⁶ In other words, no aluminum nor boron bound exciton luminescence was observed despite high concentrations of Al and B in the samples used. It is believed that the forward tunneling of bound excitons to In bound states is responsible for the quenching of the B and Al luminescence. Consequently, it appears that PL may not be particularly useful for determining the concentration of a second impurity in the presence of another dopant at much higher concentrations.

The main goal of this research project is to understand the electromagnetic properties of multiply-doped silicon, and, in particular, to provide a theory interpreting the experimental results on PL from the Si:(In,Al) system by Brown, et al.⁶, as well as predicting the reverse exciton tunneling for the systems Si:(B,Al), Si:(B,Ga), and Si:(Al,Ga). We do not attempt to solve the PL problem using the exact Schrödinger equation for an exciton because of its complexity; instead, we use the simplest model to obtain the PL intensity ratio for the doubly-doped semiconductor, leaving more complicated and sophisticated models for later investigations.

In the next section, we present a general PL theory for doubly-doped semiconductors; this theory takes into account forward and reverse exciton tunneling, impurity distributions, the resulting rate equations, and their steady-state solutions in the absence of saturation. We calculate in Section III the forward and reverse exciton tunneling rates using a simple model of a BE in a one-dimensional semi-infinite double potential well (OSDW) using standard methods of quantum mechanics⁷. The exciton

energy eigenvalue equation is also derived for estimating the tunneling time. In Section IV, we calculate the tunneling rate and derive the energy eigenvalue equation for a BE in a onedimensional finite double potential well (OFDW) for future use. The numerical results and discussion along with recommendations and suggestions for further work are presented in Section V.

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SECTION II

A THEORY OF PHOTOLUMINESCENCE FOR A DOUBLY-DOPED SEMICONDUCTOR INCLUDING EXCITON TUNNELING

1. IMPURITY DISTRIBUTION

To study the concentration effect on luminescence of two impurity atoms in a semiconductor, we consider here some direct interactions⁸ between an exciton bound to impurity atom "1" (A_1) and its nearest neighbor neutral impurity atom "2" (A_2) which results in tunneling of the exciton from the atom A_1 to the atom A_2 (due to overlap of the wavefunctions for the A_1 BE and A_2 BE) and its reverse tunneling. From here on, we will use the subscript "1" and "2" for quantities associated with impurity atom "1" with shallow BE energy levels and with impurity atom "2" with deep BE energy levels, respectively; e.g., N_1 = the concentration of B atoms, I_2 = the intensity of PL from the In BE, σ_1 = the FE capture cross section by impurity atom "1".

We calculate first the probability that the nearestneighbor atom A_2 is between r and r + dr from a given atom A_1 as shown in Fig. 1

$$P_{2}(r)dr = 4\pi r^{2}drN_{2} \exp[-\frac{4}{3}\pi r^{3}N_{2}]$$
(1)

where

 $4\pi r^2 drN_2$ = The probability that an atom A_2 is between r and r + dr from a given atom A_1 $exp[-\frac{4}{3}\pi r^3N_2]$ = The probability that there is no atom A_2 between the atom A_1 and r (obtained from the Poisson

distribution).

$$A_{1} = \text{Impurity Atom "1"} \\ 0 - - - - r - - + \\ No A_{2} \text{ atoms} A_{2} \\ dr \end{pmatrix} = \text{Impurity Atom "2"} \\ A_{2} \\ 0 \\ dr \end{pmatrix}$$

Figure 1. Configuration of impurity atoms in a doubly-doped semiconductor.

Note that

$$\int_{0}^{\infty} P_{2}(r) dr = 1 .$$
 (2)

The average value of r for a given A_2 concentration is

$$\langle r \rangle_2 = \int_0^\infty r P_2(r) dr = (3/4\pi N_2)^{-1/3} \Gamma(4/3)$$
 (3)

where $\Gamma(x)$ is the gamma function⁹. For $N_2 = 10^{16} \text{ cm}^{-3}$ we find $\langle r \rangle_2 = 257 \text{Å}$. Considering that the Si BE Bohr radius is 43Å, it is reasonable to assume that direct interaction effects are important.

Now the density of atoms ${\rm A}_1$ with a nearest-neighbor atom ${\rm A}_2$ between r and r+dr is given by

$$N_1(r) = N_1 P_2(r)$$
, (4)

so that

$$\int_{0}^{\infty} N_{1}(r) dr = N_{1} \int_{0}^{\infty} P_{2}(r) dr = N_{1}$$
 (5)

Simply switching the subscript $"_2$ " to subscript $"_1$ " in Eqs. (1) and (4), we obtain the probability that the nearest-neighbor atom A₁ is between r and r+dr from a given atom A₂ as well as the density of A₂ atoms.

2. THE RATE EQUATIONS AND STEADY STATE SOLUTIONS

We use a model for the formation and decay kinetics of FE and BE including forward and reverse BE tunneling to derive a formula for the relative intensity of PL from two dopants in a semiconductor as a function of their concentrations. For this purpose, we start with the rate equations for the densities of the FE and BE^8 .

$$\frac{dn_{FE}}{dt} = g - (v_{FE} + \gamma_1 + \gamma_2)n_{FE} + \rho_1 n_1 + \rho_2 n_2 , \qquad (6)$$

$$\frac{\partial n_1(r)}{\partial t} = \gamma_1(r) n_{FE} - \{v_1 + \rho_1 + \Omega_1(r)\} n_1(r) + \Omega_2(r) n_2(r) , \quad (7)$$

$$\frac{\partial n_2(r)}{\partial t} = \gamma_2(r) n_{FE} - \{ \upsilon_2 + \rho_2 + \Omega_2(r) \} n_2(r) + \Omega_1(r) n_1(r) .$$
 (8)

Here

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g	=	the free exciton (FE) generation rate
n _{fe}	=	the FE density
$^{\vee}$ FE	=	the FE decay rate
n j	=	the density of excitons bound to impurity atom
		j (j = 1 or 2); e.g., "1" = A1, "2" = In
n _i (r)	=	the density of excitons bound to impurity atom i
		with a nearest-neighbor impurity atom j (\neq i)
		between r and r + dr
γi	=	the FE capture rate by impurity atom i
$\gamma_{i}(r)$	=	the FE capture rate by impurity atom i with nearest-
		neighbor impurity atom j (\neq i) between r and r + dr
^v i	=	the BE _i decay rate
$^{ m ho}$ i	=	the thermal release rate of BE _i
$u_i(r)$	=	the distance dependent exciton tunneling rate from
		impurity atom i to impurity atom i $(\neq i)$.

Integrating Eq. (13) over r, we obtain

$$n_{i} = \int_{0}^{\infty} n_{i}(r) dr$$
$$= \xi_{i} n_{FE} \left\{ 1 + \frac{\gamma_{j}}{\gamma_{i}} J_{j} - J_{i} \right\}$$
(17)

where

$$J_{i} = \int_{0}^{\infty} P_{j}(r) w_{i}(r) \{1 + w_{1}(r) + w_{2}(r)\}^{-1} dr$$
 (18)

with

$$P_{j}(r) = 4\pi r^{2} N_{j} \exp(-\frac{4\pi}{3}r^{3} N_{j})$$
(1)

3. THE INTENSITY RATIO OF BOUND EXCITON LUMINESCENCE

Using Eq. (17) we have the ratio of PL intensity of $BE_{\rm i}$ to that of FE

$$\frac{I_{i}}{I_{FE}} = \frac{f_{i}n_{i}}{f_{FE}n_{FE}} = \frac{f_{i}}{f_{EF}} \xi_{i}\{1 + \frac{\gamma_{j}}{\gamma_{i}}J_{j} - J_{i}\}$$
(19)

where f_i is the BE_i oscillator strength and f_{FE} is the FE oscillator strength. With the help of Eq. (19), we have the intensity ratio of BE luminescence

$$\frac{I_{1}}{I_{2}} = R_{12} \frac{N_{1}}{N_{2}} , \qquad (20)$$

where

$$R_{12} = R_{12}^{(0)} R(1,2)$$
 (21)

with

$$R_{12}^{(0)} = \frac{f_1}{f_2} \left\{ \frac{\xi_1 N_2}{\xi_2 N_1} \right\} = \frac{f_1}{f_2} \frac{\sigma_1 / (\nu_1 + \rho_1)}{\sigma_2 / (\nu_2 + \rho_2)}$$
(22)

= the value of R₁₂ in the absence of
exciton tunneling,

$$R(1,2) = \frac{1 + \eta^{-1} \cdot J_2 - J_1}{1 + \eta \cdot J_1 - J_2}$$
(23)

and

$$= \frac{\gamma_1}{\gamma_2} = \frac{\sigma_1 N_1}{\sigma_2 N_2} \qquad (24)$$

We name R(1,2) in Eq. (23) the "tunneling factor" of a bE from impurity 1 to impurity 2. It has the following characteristics: no BE tunneling will occur if R(1,2) = 1, the forward BE tunneling from the shallow impurity to the deep impurity dominates if R(1,2) < 1, and the reverse BE tunneling from the deep impurity to the shallow impurity dominates if R(1,2) > 1. We point out here that Eq. (21) contains the vital information on PL from a doubly-doped semiconductor which depends on the impurity concentrations as well as parameters such as the FE and BE oscillator strengths and the FE capture cross sections.



SECTION III

TUNNELING RATE AND ENERGY EIGENVALUE EQUATION FOR AN EXCITON IN A ONE DIMENSIONAL SEMI-INFINITE DOUBLE POTENTIAL WELL

Before we compare this theory with the experimental results, we must calculate the exciton tunneling rates $\Omega_i(r)$ in Eqs. (16), (18), and (23). The general topic of tunneling in solids has been considered extensively in the literature^{10,11}.

1. TUNNELING RATE CALCULATION

Here we treat the exciton, a correlated electron-hole pair, as a single particle and assume that it moves in a OSDW, as shown in Fig. 2. It is assumed that the exciton is initially in potential well "1" (Region I in Fig. 2).



Figure 2. An exciton in one-dimensional semi-infinite double potential well (OSDW).

The motion of an exciton with effective mass m in the potential well shown in Fig. 2 is governed by the Schrodinger equation

$$\frac{\hbar^2}{2m} \frac{d^2 \Psi}{dx^2} + (E - V) \Psi = 0 , \qquad (25)$$

with the solutions

$$\Psi_{I}(\mathbf{x}) = Ae^{\mathbf{i}k_{1}\mathbf{x}} + Be^{-\mathbf{i}k_{1}\mathbf{x}} , \qquad 0 \leq \mathbf{x} \leq \mathbf{a}_{1}$$

$$\Psi_{II}(\mathbf{x}) = Ce^{-\kappa\mathbf{x}} + De^{\kappa\mathbf{x}} , \qquad \mathbf{a}_{1} \leq \mathbf{x} \leq \mathbf{a}_{1} + \mathbf{b} \qquad (26)$$

$$\Psi_{III}(\mathbf{x}) = Ee^{\mathbf{i}k_{2}\mathbf{x}} , \qquad \mathbf{a}_{1} + \mathbf{b} \leq \mathbf{x} \leq \mathbf{a}_{1} + \mathbf{a}_{2} + \mathbf{b}$$

where

$$k_{i} = \sqrt{2m(V_{i} - E)/\hbar}$$

$$\kappa = \sqrt{2mE/\hbar}$$
(27)

and constants A, ...E are to be determined by the boundary conditions. The boundary conditions between regions I and II, and II and III yield

$$E/A = 4i\zeta_{1}e^{i(z_{1}-z_{1})}/\Delta_{1}$$

$$L_{1} = e^{-\epsilon b}(1 + i\zeta_{1})(1 + i\zeta_{2}) - e^{\kappa b}(1 - i\zeta_{1})(1 - i\zeta_{2}) \quad (28)$$

$$u_{i} = k_{i}a_{i} , \qquad c' = k_{2}(a_{1} + b) , \qquad \zeta_{i} = k_{i}/\kappa$$

A transmission coefficient T can be calculated by taking the ratio of the current density of particles transmitted through the barrier, J_{III} , and the incident current density, J_{I} ,

$$T = J^{III} / J_{I} = (k_{2} / k_{1}) (E/A)^{2}$$
(29)
= $rk_{1}k_{2}\kappa^{2} / \Delta$
$$\Delta = \kappa^{4} |\Delta_{1}|^{2} / 4$$

= $(k_{1}^{2} + \kappa^{2}) (k_{2}^{2} + \kappa^{2}) \sinh^{2}(\kappa b) + \kappa^{2} (k_{1}^{2} + k_{2}^{2})$

The tunneling rate from well "1" to well "2" is defined as the transmission coefficient divided by the period of classical oscillations within potential well "1":

$$\Omega_{1}(r) = T/(2ma_{1}/k_{1})$$

$$= \Omega_{1} e^{-2\kappa r}$$

$$= \frac{2hk_{1}}{ma_{1}} \frac{4k_{1}k_{2}\kappa^{2}}{(k_{1}^{2} + \kappa^{2})(k_{2}^{2} + \kappa^{2})} e^{2\kappa(a_{1}+a_{2})}$$

$$r = a_{1} + a_{2} + b .$$
(30)

where

 $\Omega_{\mathbf{1}}$

In arriving at Eq. (30), we have ignored the term with $e^{-\kappa D}$ in Eq. (29) assuming a large separation of two wells. The reverse tunneling rate is obtained by exchanging subscripts 1+2 in Eq. (30) multiplied by a Boltzmann factor exp (- $\Delta E/kT$) with $\Delta E = E_1 - E_2$ (the difference in the BE energy levels in two wells.

The tunneling rate from impurity atom A_1 to impurity atom A_2 by Eq. (30) is overestimated for the approximate concentration range below $N_2 = 10^{17} \text{ cm}^{-3}$ for the actual three-dimensional problem. We discuss below how to remedy this problem. It is reasonable to assume that 12 impurity atoms A_2 are distributed at equi-distance $< r <_2$ from each other on the spherical shell of radii $< r >_2$ and $< r <_2 + dr$ centered at the atom A_1 , which is analogous

to a close hexagonal packing of atoms in a solid. The total width of the potential wells of the 12 impurity atoms A_2 on the shell does not occupy the entire region of the spherical shell, if the concentration of the atoms A_2 is less than approximately 10^{17}cm^{-3} . Taking account of this fact, the more accurate expression for the tunneling rate is given by

$$\Omega_{1}^{(3)} = C_{1}\Omega_{1}(r)$$
 (31)

where

$$C_{1} = 6 \left[1 - \sqrt{1 - (a_{2}/(r)_{2})^{2}} \right] = 6 \left[1 - \sqrt{1 - \frac{a_{2}}{\Gamma(\frac{4}{3})} (\frac{4\pi N_{2}}{3})^{1/3}} \right]^{2}$$

for $N_{2} \approx 10^{17} \text{ cm}^{-3}$ (32)
 $C_{1} = 1$ for $N_{2} \approx 10^{17} \text{ cm}^{-3}$

For concentrations greater than about 10^{17} cm⁻³, the correction factor C₁ becomes unity due to overlap of the potential wells.

The relationship between the depth, width, and the energy eigenvalue for the exciton in an isolated semi-infinite well is given by

$$\tan(k_i a_j) + k_j / \kappa = 0$$
 (33)

We assume that the reverse tunneling from well "2" to well "1" will take place after the exciton in well "2" is raised from its deeper energy level E_2 to a shallower energy level E_1 by thermal excitation.

The tunneling rate may be calculated by various other means: e.g. the semiclassical approximation by Wentzel, Kramers, and Brillouin (the WKB approximation)⁷ yields a tunneling rate similar to Eq. (30). In general, the tunneling rate depends on a dominant factor $exp(-2\kappa r)$ regardless of the model used because the wavefunction representing a BE behaves as $exp(-\kappa r)$ after tunneling through a potential barrier.

2. DERIVATION FOR THE ENERGY EIGENVALUE EQUATION

Here we derive the energy eigenvalue equation for an exciton in an OSDW in order to compute the BE₁ tunneling time. The wavefunctions in the three regions which satisfy the appropriate boundary conditions are

$$\Psi_{I} = A' \sin(k_{1}x)$$

$$\Psi_{II} = B'e^{-\kappa x} + C'e^{\kappa x}$$

$$\Psi_{III} = D' \sin(k_{2}(a_{1} + a_{2} + b - x))$$
(34)

By eliminating the constants A', B', C', and D' from the four equations for the boundary conditions $(\Psi_{I}(a_{1}) = \Psi_{II}(a_{1}), \Psi_{I}(a_{1}) = \Psi_{II}(a_{1}); \Psi_{II}(a_{1} + b) = \Psi_{III}(a_{1} + b), \Psi_{II}'(a_{1} + b) = \Psi_{III}'(a_{1} + b), we have the exciton energy eigenvalue equation$

$$F_1 F_2 = e^{-2\kappa b}$$
(35)

$$= \frac{\tan(k_i a_i) + k_i/\kappa}{\tan(k_i a_i) - k_i/\kappa}$$
(36)

where

Equation (35) reduces to Eq. (33) for a large separation, b, of the two wells.

F_i

SECTION IV

TUNNELING RATE AND ENERGY EIGENVALUE EQUATION FOR AN EXCITON IN ONE DIMENSIONAL FINITE DOUBLE POTENTIAL WELL

We give here the tunneling rate of an exciton in a OFDW and the energy eigenvalue equation for future use. The exciton tunneling rate is

$$u_{1}(\mathbf{r}) = \Omega_{1}' e^{-2\kappa \mathbf{r}}$$

$$u_{1}' = \Omega_{1} e^{-\kappa (a_{1} + a_{2})}$$

$$\mathbf{r} = \frac{1}{2}(a_{1} + a_{2}) + \mathbf{b}$$
(37)

The realistic tunneling rate is obtained by multiplying Eq. (37) by the correction factor given in Eq. (32) as in the case for the OSDW.

The energy eigenvalue equation is

$$G_1 G_2 = e^{-2\kappa b}$$
(38)

where

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$$G_{i} = \left\{ 2\cot(k_{i}a_{i}) - \left(\frac{k_{i}}{\kappa} - \frac{\kappa}{k_{i}}\right) \right\} / \left\{ \frac{k_{i}}{\kappa} + \frac{\kappa}{k_{i}} \right\}$$

$$= \left\{ 1 - \frac{k_{i}}{\kappa} \tan\left(\frac{k_{i}a_{i}}{2}\right) \right\} \left\{ 1 + \frac{\kappa}{k_{i}} \tan\left(\frac{k_{i}a_{i}}{2}\right) \right\} / \tan\left(\frac{k_{i}a_{i}}{2}\right) \left\{ \frac{k_{i}}{\kappa} + \frac{\kappa}{k_{i}} \right\}$$
(39)

SECTION V NUMERICAL RESULTS AND DISCUSSIONS

It is convenient to introduce the forward tunneling coefficient w_i (= w_{ij}) which is defined by

$$\mathbf{w}_{i} = \mathbf{w}_{ij} = \Omega_{i} / (\nu_{i} + \rho_{i})$$
(40)

where $(v_i + \rho_i)$ is the total decay rate of BE_i, i.e., the sum of the BE_i decay rate and thermal release rate of BE_i , each of which is estimated using the experimental value of the BE lifetime at 4.2K.^{5,12} It turns out that v_i , the thermal release rate, is negligible for all cases with the exception of the BE for boron at this temperature. We have used the experimental values of ionization energies determined by Lipari et al.¹³ to estimate the BE ionization energies with the help of the Haynes rule. There are still four parameters a_1 , a_2 , V_1 , and ${\rm V}_2$ (the widths and depths of the two potential wells) to be determined before calculating the tunneling coefficients; however, the energy eigenvalue equation for each separate well (Eq. (33)) effectively reduces the number of unknowns to two. For the system Si:(B,In), we have fixed the numerical value of one parameter, a_p, to match the values of R(B,In) obtained by Mitchard and McGill⁵ for the boron concentration range N_R = 10^{12} - 10^{14} cm⁻³ and the indium concentration range $N_{In} = 10^{12} - 10^{15} cm^{-3}$ and approximated the other, a_{Tn} , as the first Bohr radius in the context of the hydrogenic BE model. For the rest of the systems, we have determined the shapes of the potential wells using a similar process. The numerical values of the BE ionization energy (E), wavenumber (κ) , potential depth (V), potential width (a), total decay rate (v+p), forward tunneling coefficient (w_{ij}) and reverse
tunneling coefficient (w_{ji}) for each system are summarized in Table 1 for the BE model presented in Section III (an exciton in a OSDW).

Note here that the reverse tunneling coefficients w_{ji} are calculated with the help of Eq. (40) exchanging the subscript i \leftrightarrow j multiplied by the Boltzmann factors. As seen in Table 1, the reverse tunneling coefficients w_{ji} for the systems Si:(B,In), Si:(Al,In) and Si:(Ga,In) are extremely small and thus neglected for evaluating their tunneling factors R(i,j).

With few exceptions, the FE capture cross sections by neutral acceptors in silicon are not well known. We take $\sigma_{\rm B}/\sigma_{\rm In}$ = 0.1 ^{5,14} for the system Si:(B,In). For the system Si:(Al,In), we have estimated $\sigma_{Al}/\sigma_{In} = 1.4$, using a linear relationship between the reciprocal of the FE capture time¹⁵ and the FE capture cross section. However, we also examine four other values 0.05, 0.2, 5, and 20 for $\sigma_{\rm Al}^{}/\sigma_{\rm In}^{}$ to evaluate the tunneling factor R(Al, In) because of uncertainty in the FE capture cross section ratio. We use the same set of values for the $\sigma^{}_{\rm Ga}/\sigma^{}_{\rm In}$ rate in the system Si:(Ga,In) as that for the system Si: (Al, In) because aluminum and gallium have similar electronic properties in Si. For the systems Si: (B,Al) and Si: (B,Ga), we take the set of values 0.005, 0.02, 1/14, 0.5, 2, and 20 for their FE capture cross section ratios. Finally, for the system Si:(Al,Ga), we examine values of 0.05, 0.2, 1, 2, 10, and 50 for the σ_{Al}/σ_{Ga} ratio.

TABLE 1

BOUND EXCITON IONIZATION ENERGIES, WAVENUMBERS, POTENTIAL DEPTHS, POTENTIAL WIDTHS, TOTAL DECAY RATES, FORWARD AND REVERSE TUNNELING COEFFICIENTS

^w BGa ^w AlGa) (10 ¹⁰) (10 ¹⁰)	125.89	7* 14.61	0.01770* 6.178*	
In ^w BAl 10) (10 ¹⁰	174.0	0.059	612	4 x -12*
AlIN ^w Ga 10 ¹⁰) (10		2635	0.2	96 x 7.97
w _{BIn} w (10 ¹⁰) (3.966	0.		1.406 x 3.2 10 ⁻¹⁴ * 1
v + p (10 ⁶ s ⁻¹)	1.270	13.23	13.02	370.4
a (Å)	160.0	98.0	92.0	34.0
v (meV)	6.377	11.43	12.33	44.67
к (10 ⁶ cm ⁻¹)	2.580	3.198	3.281	4.774
E (meV)	4.583	7.042	7.416	15.694
Impurity	щ	Al	Ga	In

* The reverse tunneling coefficients w_{ji} are calculated with the help of Eq. (40) exchanging the subscript i + j multiplied by the Boltzmann factor.

ions for the tunneling factor are plotted in Fig. 3a, as of $N_{\rm B}$ (10¹²-10²⁰ cm⁻³). nt views of the three dimensional $N_{\rm B}$ and $N_{\rm Tn}$. Similar plots for by Mitchard and McGill⁵ are n. For the boron concentration the indium concentration range ineling factors R(B,In) and each other because the potential Si:(B,In) have been chosen to above concentration ranges. ve ranges, however, R(B,In) ses more rapidly than R_{mm}(B,In) e tunneling coefficient of that of 10⁷ by Mitchard and in the exponential factor for the

In other words, the present ling rate and thus stronger luminescence than that predicted centrations below 10¹⁴ cm⁻³, both ity which implies no BE tunneling

. 3b, 3c, 4b, and 4c indicate
(B,In) = 1).
1) for the system Si:(Al,In)
cross section ratios of
20 and are plotted in Figs.

5a-9c. For all the values of σ_{Al} no BE tunneling if both aluminum less than 10^{14} cm^{-3} . Comparison c $\sigma_{Al}/\sigma_{In} = 0.05$) and 9a (R(Al,In) there is more BE tunneling at a g larger value of σ_{Al}/σ_{In} . In Tabl $R^{(O)}$ (Al,In) and the tunneling fac σ_{Al}/σ_{In} for $N_{Al} = 3.03 \times 10^{15} \text{ cm}^{-3}$ in order to compare the theory and et al.⁶ The values of $R^{(O)}$ (Al,In using the relative oscillator street et al.¹⁶ The theory predicts vertex

TABLE

 $R^{(O)}(Al,In)$ AND R(Al,In)FOR $N_{Al} = 3.03 \times 10^{15} cm^{-3}$ AN

^o Al ^{/o} In	0.05	0.2
$R^{(o)}$ (Al, In)	0.0875	0.350
R(A1,In)	0.000537	0.000534

factors for the above concentratio the help of Eqs. (20) and (21), th the system Si:(Al,In) is

$$\frac{I_{A1}}{I_{In}} = R^{(0)} (A1, In)$$

Referring to Table 2, Eq. (41) giv relative PL intensity

$$\frac{I_{A1}}{I_{TP}} = 3.57 \times 10^{-4}$$
 (42)

which is still below the sensitivity of the experiment to observe PL from aluminum. Thus it confirms the experimental results by Brown et al.⁶ that no aluminum BE luminescence should be observed at these concentrations.

The tunneling factors R(Ga,In) for the system Si:(Ga,In) are calculated for the $\sigma_{Ga}/\sigma_{In} = 0.05$, 0.2, 1.4, 5, and 20 and plotted in Figs. 10a-14c. These figures are very similar to those for the system Si:(Al,In), i.e. they indicate no BE tunneling from gallium to indium if the concentrations are below 10^{14} cm⁻³, and strong quenching of gallium bound exciton luminescence for In concentrations beyond 10^{17} cm⁻³.

For the systems Si:(B,Al) and Si:(B,Ga), we have calculated the tunneling factors R(B,Al) and R(B,Ga) for the FE capture cross section ratios $\sigma_{B}/\sigma_{A1} = \sigma_{B}/\sigma_{Ga} = 0.005, 0.02, 1/14, 0.5, 2, and$ 20, and plotted them in Figs. 15a-20c and Figs. 21a-26c, respectively. The figures corresponding to the same FE capture cross section are very similar to each other. Once again they show no BE tunneling from the shallow impurity to the deep impurity if their concentrations are below 10^{14} cm⁻³. For $\sigma_{\rm B}/\sigma_{\rm A1} = \sigma_{\rm B}/\sigma_{\rm Ga} = 0.005$, however, Figs. 15a and 21a show very little quenching of boron bound exciton luminescence and rather an enhancement if $N_{\rm B} < 10^{14} {\rm cm}^{-3}$, $N_{\rm Al} > 10^{16} {\rm cm}^{-3}$ and $N_{\rm Ga} > 3 {\rm x} 10^{16} {\rm cm}^{-3}$. The finite values of the reverse tunneling coefficients are responsible for this phenomenon (see Table 1). In other words, for a small value of the FE capture cross-section ratio, the reverse tunneling from the deeper impurity to the shallower impurity starts to dominate the forward tunneling from the shallower

impurity to the deeper impurity for the above concentrations, resulting in only slight quenching of the shallow impurity bound exciton luminescence. For $\sigma_{\rm B}/\sigma_{\rm Al} = \sigma_{\rm B}/\sigma_{\rm Ca} = 20$, Figs. 20a and 26a show considerable quenching of boron bound exciton luminescence if $N_{\rm B} < 10^{14} {\rm cm}^{-3}$ and $N_{\rm Al} = N_{\rm Ga} = 3 \times 10^{16} {\rm cm}^{-3}$ and enhancement if $N_{\rm B} < 10^{14} {\rm cm}^{-3}$ and the extremely high concentrations of $N_{\lambda 1} = N_{Ga} = 10^{20} \text{ cm}^{-3}$. For a large value of the FE capture crosssection ratio, a large number of excitons are captured by the shallower impurity, most of them are lost to the deeper impurity via forward BE tunneling, and the smaller number of excitons captured by the deeper impurity stay there because of the small reverse BE tunneling coefficients, if $N_{\rm R} < 10^{14} {\rm cm}^{-3}$ and $N_{\rm Al}$ = $N_{Ca} = 3 \times 10^{16} \text{ cm}^{-3}$. Thus considerable quenching of boron bound exciton luminescence occurs at these concentrations. For the extremely high concentrations of $N_{A1} = N_{Ga} = 10^{20} \text{ cm}^{-3}$, the reverse tunneling from the deeper impurity to the shallower impurity starts to dominate the forward tunneling and enhances the shallower impurity bound exciton luminescence. Once again, the plateau regions of Figs. 155,c - 26b,c indicate the regions exhibiting no BE tunneling.

The results of the calculations for the tunneling factors R(AI,Ga) for the system Si:(Al,Ga) with the FE capture cross-section ratios $r_{AI}/r_{Ga} = 0.05$, 0.2, 1, 2, 10, and 50 are plotted in Figs. 27a - 32c. Figures 27a and 28a show no quenching of aluminum bound exciton luminescence and its enhancement if $N_{AI} \sim 10^{14} \text{ cm}^{-3}$ and $N_{Ge} < 3 \times 10^{15} \text{ cm}^{-3}$ due to the fact that the forward and reverse tunneling coefficients are of the same order of magnitude and the difference in their BE energy levels is very

small. For $\circ_{A1}/\circ_{Ga} \sim 1$, slight quenching of aluminum bound exciton luminescence occurs at certain gallium concentrations; e.g. $N_{Ga} = 3 \times 10^{15} \text{ cm}^{-3}$ for $\sigma_{A1}/\sigma_{Ga} = 1$ and $N_{Ga} = 3 \times 10^{16} \text{ cm}^{-3}$ for $\circ_{A1}/\circ_{Ga} = 50$ (see Figs. 29a and 32a). Figs. 29a and 32a also show enhancement of aluminum bound exciton luminescence if $N_{Ga} \geq 10^{16} \text{ cm}^{-3}$ for $\circ_{A1}/\circ_{Ga} = 1$ and $N_{Ga} \geq 6 \times 10^{17} \text{ cm}^{-3}$ for $\circ_{A1}/\circ_{Ga} = 50$, because the reverse tunneling starts to dominate beyond these concentrations.

Finally, to ensure the occurrence of BE tunneling, we have estimated the tunneling time of a BE from one potential well to another for the system Si:(B,In) at $N_{In} = 10^{16} \text{ cm}^{-3}$ by two different methods:

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- 1. The reciprocal of the tunneling rate (Eq. (30)) gives the tunneling time of 1.14×10^{-11} s.
- 2. Eq. (35) with the help of time-dependent perturbation theory yields the tunneling time of 1.10×10^{-11} s. Since the tunneling time at $N_{\rm In} = 10^{16} {\rm cm}^{-3}$ is much less than the boron BE decay time of 10^{-6} s (Auger lifetime)^{12,17}, BE tunneling will occur before decay.

We summarize the results of the present calculation by pointing out that PL can be used as a quantitative tool to measure the impurity concentrations in a doubly doped semiconductor if their concentrations are less than 10¹⁴ cm⁻³ because the theory predicts no BE tunneling for all the systems considered here. As a result, PL can be an excellent quantitative tool for evaluating high purity silicon production and processing steps such



as silane and polycrystalline Si purity analysis, as well as monitoring the compositions of epitaxial silicon films. The silicon materials industry is currently exploiting the PL technique for these purposes.

We conclude this section with the following recommendations and suggestions:

1. In order to confirm the predicted reverse BE tunneling from a deeper impurity to a shallower impurity when there is a small difference in their ionization energies, we recommend, for example, measuring the relative PL intensity I_B/I_{Ga} at $N_B =$ 10^{13} cm⁻³ and $N_{Ga} = 10^{17} - 10^{18}$ cm⁻³ for the system Si:(B,Ga) or the corresponding Si:(B,Al) system.

2. Since, as indicated in Eq. (23), the tunneling factor R(1,2) strongly depends on the FE capture cross-section ratio, σ_1/σ_2 , it would be very useful to measure and/or calculate that ratio accurately, perhaps using a model analogous to positronium capture by a neutral atom.

3. Historically, minority lifetime killer dopants, e.g. zirconium¹⁸ have been added to Si in an attempt to improve detector performance in radiation environments. It is possible that, for excitons in Si, a deep acceptor could play an analogous role in a more benign fashion.

4. Since current silicon growth and processing technology has not yet reached the point where all defects save the major dopants are eliminated, it would be a valuable extension of this work to consider the exciton tunneling problem in a multi-component material. Also, due to the increased attention devoted to Si counter-doped extrinsic detectors, it would be useful to evaluate

compensation effects by appropriately including donor bound exciton capture and transfer in the rate equations used in this model. These modifications, while useful in assessing the viability of PL in quantitative determinations of physically realistic materials, are outside the scope of the present investigation.

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NOTE TO ACCOMPANY FIGURES 3 THROUGH 32

The range of the concentrations, N_i , of each of two impurities in silicon is $10^{12} - 10^{20} \text{ cm}^{-3}$. The letter "a" immediately following a figure numeral refers to the two dimensional plot of the tunneling factors R(i,j) for a given free exciton capture cross section ratio for the system Si:(i,j) as a function of the concentration N_j of impurity j for the given concentrations N_i of impurity i. The letters "b" and "c" immediately following a figure numeral refer to two different views of the three-dimensional plot of the tunneling factor R(i,j) for a given free exciton capture capture cross-section ratio as a function of N_i and N_j .













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20 as functions of $^{\rm N}{}_{\rm A\,l}$ for given N Н AI Figure 20a. R(B,Al) for '_{B'}

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