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Effect of bulk inversion asymmetry on [001], [110], and [111] GaAs/AlAs quantum wells

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The spin splitting of the conduction band due to the inversion asymmetry of the microscopic crystal potential is predicted to depend linearly on the components of the parallel wave number $\mathbf{k}_\parallel$ for small $k_\parallel$ in undoped GaAs/AlAs quantum wells. The linear dependence is due to the quantization of the confinement levels; the bulk spin splitting depends cubically on $\mathbf{k}$. We have calculated the splitting both numerically and analytically for GaAs/AlAs quantum wells grown along the [001], [110], and [111] directions. In the linear regime the average spin splitting is shown to be about a factor of 2 smaller for [110] quantum wells than for [001]- and [111]-grown quantum wells. The splitting is calculated to be $\Delta E = 4$ meV at $k_\parallel = 0.07(2\pi/a)$ for a 25-Å [001]-grown GaAs/AlAs quantum well.

Spin splittings of energy bands of zinc-blende semiconductor modulation-doped heterostructures and quantum wells have been extensively studied both experimentally[1] and theoretically.[2] The splittings are then caused by the inversion asymmetry of the macroscopic, i.e., slowly varying on the scale of the lattice parameter a, interface, or confinement potential. Homogeneous zinc-blende semiconductors exhibit an intrinsic spin splitting due to the inversion asymmetry of the microscopic crystal potential.[3] As a result terms linear in $k \equiv |\mathbf{k}|$ may appear in the valence-band structure, but calculations of Cardona, Christensen, and Fasol[4] show and that the corresponding splittings are extremely small, < 1 meV, for zinc-blende semiconductors. In addition terms cubic in k may occur both in the conduction band and the valence bands. They are associated with Kane's[3] B parameter and are not all that small. Christensen and Cardona[5] obtain a theoretical estimate of 75 meV for the maximum splitting in GaAs occurring for $\mathbf{k}$ along [110]. Effects of this splitting have been observed in spin-polarized photoemission,[6] the Hanle effect,[7] and infrared spin resonance.[8]

This Rapid Communication addresses the effects of the inversion asymmetry of the microscopic crystal potential in undoped GaAs/AlAs quantum wells grown along the [001], [110], and [111] directions, i.e., in systems having a macroscopic inversion-symmetric confinement potential. We show that the spin splitting depends linearly on the components of the parallel wave number $\mathbf{k}_\parallel$ for small $k_\parallel$ ($\equiv |\mathbf{k}_\parallel|$) and calculate its magnitude both numerically and analytically as a function of $\mathbf{k}_\parallel$; the crystal-momentum-like quantum number $\mathbf{k}_\parallel$ describes the translational symmetry in the parallel plane of the quantum well.

We derive a $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian for the conduction bands of bulk zinc-blende semiconductors, which reproduces their spin splittings, and develop the corresponding envelope function formalism for the quantum well consisting of these semiconductors. Perturbation theory is used to obtain analytical expressions for the spin splitting occurring in the energy spectrum of the quantum wells as a function of $\mathbf{k}_\parallel$. In these expressions contributions both linear and cubic in $k_\parallel$ appear. Their origin is discussed.

We first derive an envelope function formalism for the conduction bands of [001] grown GaAs/AlAs and alike (type-I) quantum wells which includes the spin splitting due to the inversion asymmetry of the microscopic potential. We proceed along the lines of our earlier work and omit details.[9] For each bulk constituent l ($l = W$ for the well and $l = B$ for the barrier) we expand the conduction-band wave function $\psi^l_{\mathbf{k}_\parallel}(\mathbf{r})$ into s-like spin-up ($u^l_\uparrow = |s_l\uparrow\rangle$) and spin-down ($u^l_\downarrow = -|s_l\downarrow\rangle$) conduction-band Γ-point states as

$$\psi^l_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel}[F^l_{\uparrow\mathbf{k}_\parallel}(z)u^l_\uparrow(\mathbf{r}) + F^l_{\downarrow\mathbf{k}_\parallel}(z)u^l_\downarrow(\mathbf{r})] \ , \qquad (1)$$

where the envelope vector function $\mathbf{F}^l_{\mathbf{k}_\parallel} \equiv (F^l_{\uparrow\mathbf{k}_\parallel}(z), F^l_{\downarrow\mathbf{k}_\parallel}(z))$ satisfies the Schrödinger equation $(\underline{H}^l_{\mathbf{k}_\parallel} - E^l_{\mathbf{k}_\parallel}\underline{I})\mathbf{F}^l_{\mathbf{k}_\parallel} = 0$; z is along the growth direction of the quantum well. The Hamiltonian matrix $\underline{H}^l_{\mathbf{k}_\parallel}$ can be obtained from the eight-band Kane-type $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian[9] by Löwdin renormalization[10] and the omission of $O(k^4)$ terms and is given by

$$\underline{H}_{\mathbf{k}_\parallel} = \begin{vmatrix} E_c + \tilde{e} + \frac{\gamma}{2}\tilde{k}_z(k_x^2 - k_y^2) & \frac{\gamma}{2}[\tilde{k}_z^2(k_x + ik_y) - ik_xk_y(k_x - ik_y)] \\ \frac{\gamma}{2}[\tilde{k}_z^2(k_x - ik_y) + ik_xk_y(k_x + ik_y)] & E_c + \tilde{e} - \frac{\gamma}{2}\tilde{k}_z(k_x^2 - k_y^2) \end{vmatrix} . \qquad (2)$$

Here and in the following, when confusion is unlikely we have omitted the superscript l. The energy E_c is the energy at the bottom of the conduction band, the "energy operator" $\tilde{e} = \hbar^2/2m^*(k_x^2 + k_y^2 + \tilde{k}_z^2)$, m^* is the Γ-point conduction-band effective electron mass, γ is the spin-splitting parameter as defined by Christensen and Cardona,[5] and $\tilde{k}_z$ is the operator id/dz. Setting $\mathbf{F}_{\mathbf{k}_\parallel} \propto e^{ik_z\cdot z}$ the two energy eigenvalues of the Schrödinger equation clearly exhibit the bulk spin splitting and are given by $E_{\mathbf{k}\pm} = \hbar^2k^2/2m^* \pm \gamma/2[k^2(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2) - 9k_x^2k_y^2k_z^2]^{1/2}$. The spin splitting is cubic in the components of $\mathbf{k}$ and attains a maximum value $(\gamma/2)k^3$ for $\mathbf{k}$

along the [110] direction; it is zero for $\mathbf{k}$ along [001] and [111].

The envelope function formalism developed for bulk zinc-blende semiconductors can now be suitably modified to describe type-I quantum wells. We must join the envelope functions $\mathbf{F}^W_{\mathbf{k}_\parallel}$ of the well W and $\mathbf{F}^B_{\mathbf{k}_\parallel}$ of the barrier B across the interfaces. We take the usual boundary conditions,[9,11] i.e., continuity, $\mathbf{F}^W_{\mathbf{k}_\parallel}=\mathbf{F}^B_{\mathbf{k}_\parallel}$, and "differentiability" $[\underline{A}^W(\partial/\partial z+\frac{1}{2}\underline{B}^W]\mathbf{F}^W_{\mathbf{k}_\parallel}=[\underline{A}^B(\partial/\partial z)+\frac{1}{2}\underline{B}^B]\mathbf{F}^B_{\mathbf{k}_\parallel}$, at each interface. The matrices $\underline{A}^l$ and $\underline{B}^l$ depend on $\mathbf{k}_\parallel$ and are defined by the following decomposition of Hamiltonian: $\underline{H}^l=\underline{A}^l(\partial^2/\partial z^2)+\underline{B}^l(\partial/\partial z)+\underline{C}^l$. Confined states are obtained by specifying the boundary conditions for $z\rightarrow\pm\infty$: $\lim_{z\rightarrow\pm\infty}\mathbf{F}_{\mathbf{k}_\parallel}(z)=0$.

We solve the Schrödinger equation plus boundary conditions for a quantum well of width w numerically. At a sought confinement energy $E_{\mathbf{k}_\parallel}$ we determine the four $k^l_z(E_{\mathbf{k}_\parallel})$ values and the corresponding eigenvector functions $\mathbf{F}^l_{\mathbf{k}_\parallel}(z)$ which satisfy the Schrödinger equation in each constituent l of the quantum well. Note that for $\gamma^B\neq 0$ the four $k^B_z(E_{\mathbf{k}_\parallel})$ values in the barrier are not just imaginary, but complex numbers. The quantum-well envelope vector function is then written as a linear combination of these eigenvector functions. Application of the boundary conditions yields the confinement energy.

Our formalism can also be applied to type-I quantum wells grown along the [110] and [111] directions. If the rotation from $z=[001]$ to $z'=[110]$ or [111] is governed by the orthogonal transformation $\mathbf{r}'=O\mathbf{r}$, all we have to do is apply the same rotation to $\mathbf{k}=(\mathbf{k}_\parallel,k_z)$. We obtain $\underline{H}(\mathbf{k}')=\underline{H}(\mathbf{k}=O^T\mathbf{k}')$; k'_z is along the quantum-well growth direction and $\mathbf{k}'_\parallel$ in the quantum-well plane.[12] The determination of the boundary conditions is now carried through for the primed variables. In solving the envelope function problem for non-[001]-grown quantum wells a problem arises since $\underline{H}$ now depends on $(k'_z)^3$. We omit the corresponding spurious solutions[9] and the effect of the $(k'_z)^3$ term on the boundary conditions.[13] In the following the primes are omitted.

We can also derive analytical results for the spin splitting in a quantum well. For $\mathbf{k}_\parallel=0$ the eigenstates are doubly degenerate as a result of time-reversal symmetry: no spin splitting exists. For $\mathbf{k}_\parallel\neq 0$ analytical expressions for the spin splitting can be obtained by the application of degenerate perturbation theory. The Hamiltonian is decomposed as $\underline{H}=\underline{H}_0+\underline{H}_p$ where $\underline{H}_0=(E_c+\tilde{e})\underline{I}$ and $\underline{H}_p$ contains the remaining, i.e., the γ-dependent terms. In $\underline{H}_0$ the two spin bands are decoupled and the standard single-band spin-degenerate quantum-well model is obtained.[9] The two degenerate envelope functions $\mathbf{F}^{(1)}_{\mathbf{k}_\parallel}\equiv(F_{\mathbf{k}_\parallel}(z),0)$ and $\mathbf{F}^{(2)}_{\mathbf{k}_\parallel}\equiv(0,F_{\mathbf{k}_\parallel}(z))$ at a degenerate energy $E_{\mathbf{k}_\parallel}$ obviously both satisfy $(\underline{H}_0-E_{\mathbf{k}_\parallel}\underline{I})\mathbf{F}^{(i)}_{\mathbf{k}_\parallel}=0$. The perturbation $\underline{H}_p$ results in the spin splitting $\Delta E_{\mathbf{k}_\parallel}=2(V_{11}^2+|V_{12}|^2)^{1/2}$, where $V_{ij}=\langle\mathbf{F}^{(i)}_{\mathbf{k}_\parallel}|\underline{H}_p|\mathbf{F}^{(j)}_{\mathbf{k}_\parallel}\rangle$. For [001]- and [110]-grown quantum wells V_{11} is zero and the spin splitting $\Delta E_{\mathbf{k}_\parallel}=2|V_{12}|$ can be written as

$$\Delta E_{\mathbf{k}_\parallel}=|\overline{\gamma k_z^2}(k_x+ik_y)-\bar{\gamma}ik_xk_y(k_x-ik_y)| \qquad (3)$$

for [001]-grown quantum wells where k_x and k_y are along the [100] and [010] directions, respectively, and

$$\Delta E_{\mathbf{k}_\parallel}=\frac{1}{2}\left|-\overline{\gamma k_z^2}\frac{1-i}{\sqrt{2}}k_y+\bar{\gamma}\frac{1-i}{\sqrt{2}}k_y(k_y^2-2k_x^2)\right| , \qquad (4)$$

for [110]-grown quantum wells where k_x and k_y are along the $[00\bar{1}]$ and $[\bar{1}10]$ directions, respectively. For a [111]-grown quantum well the resulting expression for the spin splitting is

$$\Delta E_{\mathbf{k}_\parallel}=\frac{1}{2\sqrt{3}}[16(\overline{\gamma k_z^2})^2(k_x^2+k_y^2)-8\bar{\gamma}\overline{\gamma k_z^2}(k_x^2+k_y^2)^2+\bar{\gamma}^2(k_x^6+21k_x^4k_y^2-9k_x^2k_y^4+3k_y^6)]^{1/2} , \qquad (5)$$

where k_x and k_y are along the $[11\bar{2}]$ and $[\bar{1}10]$ directions, respectively. The barred quantities in these expressions are defined as averages of the spin-splitting parameter γ and the confinement wave number k_z over the probability density of the confinement state, i.e., $\overline{\gamma k_z^2}=\int_{-\infty}^{+\infty}F^*_{\mathbf{k}_\parallel}(z)\times\tilde{k}_z\gamma(z)\tilde{k}_zF_{\mathbf{k}_\parallel}(z)dz$ and $\bar{\gamma}=\int_{-\infty}^{+\infty}F^*_{\mathbf{k}_\parallel}(z)\gamma(z)F_{\mathbf{k}_\parallel}(z)dz$, where the single-band envelope function $F_{\mathbf{k}_\parallel}(z)$ satisfies the normalization condition

$$\int_{-\infty}^{+\infty}F^*_{\mathbf{k}_\parallel}(z)F_{\mathbf{k}_\parallel}(z)dz=1 .$$

The integrals consist of a well contribution, a barrier contribution, and, for $\overline{\gamma k_z^2}$, of interface contributions resulting from δ singularities of $d^2F_{\mathbf{k}_\parallel}/dz^2$ and $d\gamma(z)/dz$ at the interfaces. The barred quantities depend weakly on $\mathbf{k}_\parallel$ ($<2\%$ difference for $\mathbf{k}_\parallel\in[0,0.06(2\pi/a)]$) through the weak $\mathbf{k}_\parallel$ dependence of $F_{\mathbf{k}_\parallel}(z)$. For wide wells, $w>200$ Å, $\bar{\gamma}$ and $\overline{\gamma k_z^2}$ are to within a few percent equal to γ^W and $\gamma^W(k_z^W)^2$, respectively, where k_z^W is the quantized wave number in the well.

Our model contains five parameters: the effective electron masses m^*_W and m^*_B, the spin-splitting parameters γ^W and γ^B, and the conduction-band discontinuity ΔE_c. We apply the model to GaAs/AlAs quantum wells. Thus we take $m^*_W=0.067$, $m^*_B=0.150$ and put ΔE_c equal to 0.99 eV. The spin-splitting parameter was calculated for GaAs by Christensen and Cardona[5] using the linear muffin-tin orbital (LMTO) method. We take their value, i.e., $\gamma^W=17$ eV Å^3. For AlAs no value exists. We have therefore performed an augmented spherical wave[14] (ASW) band-structure calculation for GaAs and AlAs including the spin-orbital interaction operator in the Hamiltonian.[15] Figure 1 contains our calculated results for the spin splitting of the conduction bands of GaAs and AlAs. Our results for GaAs agree with those of Christensen and Cardona to within 5%. For AlAs the spin splitting is found to have the same sign as for GaAs and it is $\approx 30\%$ smaller than that of GaAs. We consequently take $\gamma^B=12$ eV Å^3.

Figures 2–3 display our analytical results for the spin splitting of the conduction bands of 50-Å-wide [001]-, [110]-, and [111]-grown GaAs/AlAs quantum wells. We have verified that our analytical results agree with our numerical results to within 0.1%. Obviously, the spin splitting depends strongly on the growth direction of the quantum well. Unlike the bulk spin splitting which is cubic in k, it is not cubic in $k_\parallel$. Moreover, it is strongly anisotrop-

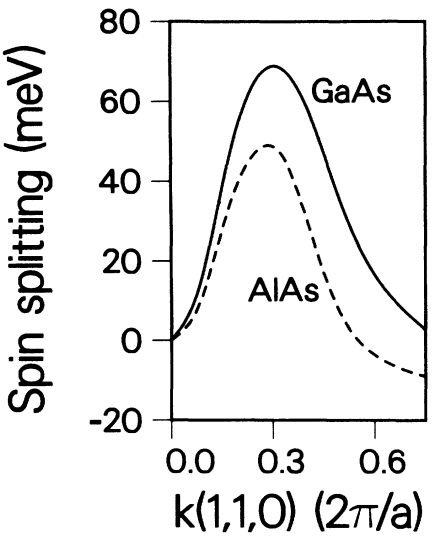

FIG. 1. Calculated ASW results for the spin splitting of the conduction bands in GaAs (solid line) and AlAs (dotted line) along $\Gamma - K$.

ic. The $\mathbf{k}_\parallel$ dependence as shown in Fig. 2 can be interpreted in detail from Eqs. (3)–(5). For small $\mathbf{k}_\parallel$, $k_\parallel \ll k_z^W$, the term containing $\overline{\gamma k_z^2}$ is dominating and the spin splitting is linear in $k_\parallel$; it is approximately equal to $\overline{\gamma k_z^2} k_\parallel$, $\frac{1}{2}\overline{\gamma k_z^2} k_y$, and $(2/\sqrt{3})\overline{\gamma k_z^2} k_\parallel$ for [001]-, [110]-, and [111]-grown quantum wells, respectively. The origin of the linear contribution in $k_\parallel$ is obvious from these formulas: It is due to the quantum-well-induced quantization of k_z in the third-order $k_z^2 k_x$ and $k_z^2 k_y$ bulk contributions. Note that

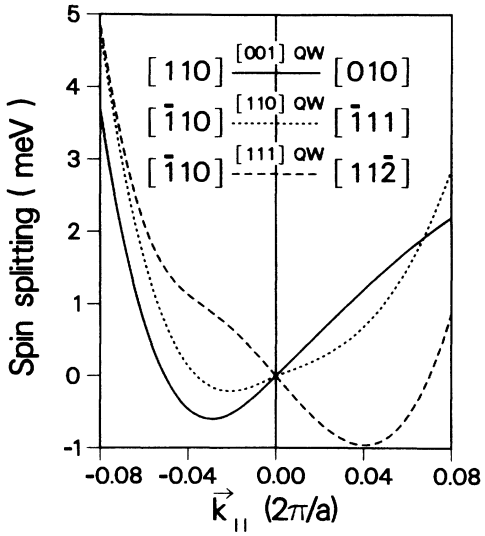

FIG. 2. Calculated [from Eqs. (3)–(5)] spin splitting of the first conduction-band confinement level for 50-Å [001]- (solid line), [110]- (dotted line), and [111]- (dashed line) grown GaAs/AlAs quantum wells. The parameters have the following values: $\bar{\gamma}=16.84$ eV Å^3 and $\overline{\gamma k_z^2}=0.028$ eV Å at $\mathbf{k}_\parallel=0$, $\bar{\gamma}=16.80$ eV Å^3 and $\overline{\gamma k_z^2}=0.025$ eV Å at $\mathbf{k}_\parallel=0.08(2\pi/a)$; cf. $\gamma=17.00$ eV Å^3 and $\gamma^W(k_z^W)^2=0.032$ eV Å.

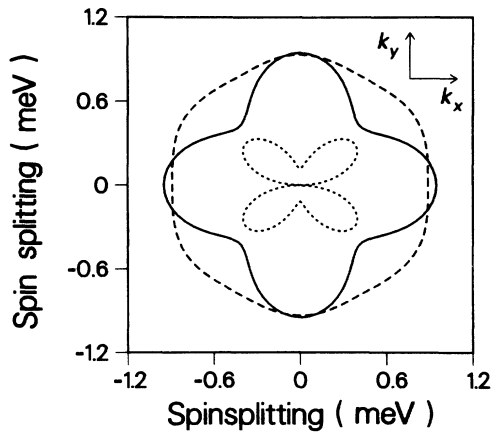

FIG. 3. Calculated [from Eqs. (3)–(5)] spin splitting of the first conduction-band confinement level for 50-Å [001]- (solid line), [110]- (dotted line), and [111]- (dashed line) grown GaAs/AlAs quantum wells for different $\mathbf{k}_\parallel=(k_x,k_y)$ directions where $k_\parallel=0.03(2\pi/a)$; k_x is along [100], [00$\bar{1}$], and [11$\bar{2}$] and k_y is along [010], [$\bar{1}$10], and [$\bar{1}$10], for [001]-, [110]-, and [111]-grown quantum wells, respectively. The parameters have the following values: $\bar{\gamma}=16.83$ eV Å^3, $\overline{\gamma k_z^2}=0.027$ eV Å, and $k_z^W=0.038(2\pi/a)$.

terms even in $k_\parallel$ do not exist because of time-reversal symmetry.

For larger $\mathbf{k}_\parallel$ the term containing $\bar{\gamma}$ in Eqs. (3)–(5) is dominating and the spin splitting is cubic in $k_\parallel$. For $k_\parallel \gg k_z^W$, the maximum value of the spin splitting occurs for $\mathbf{k}_\parallel$ along [110] for [001]-grown quantum wells and for $k_\parallel$ along [$\bar{1}$10] for both [110]- and [111]-grown quantum wells; it can be approximated by $(\bar{\gamma}/2)k_\parallel^3$. The maximum spin splitting does not depend on the growth direction and is comparable to the maximum spin splitting in the bulk $(\gamma/2)k^3$ appearing for $\mathbf{k}$ along [110]. This is not surprising since for large $k_\parallel$ the kinetic energy $(\sim\hbar^2 k_\parallel^2/2m_W^*)$ is much larger than the confinement energy $[\sim\hbar^2(k_z^W)^2/2m_W^*]$. For certain $\mathbf{k}_\parallel$ directions the spin splitting for the [001]- and [110]-grown quantum wells changes sign (see Fig. 2) due to a competition between the linear and the cubic terms in Eqs. (3) and (4). For $\mathbf{k}_\parallel=(0,k_\parallel)$, i.e., along [010], only the linear term is present for a [001]-grown quantum well and the departure from a straight line is only caused by the $\mathbf{k}_\parallel$ dependence of $\overline{\gamma k_z^2}$. In Fig. 3 the spin splitting is shown as a function of the direction of $\mathbf{k}_\parallel$ while $k_\parallel$ is kept constant. The anisotropy of the spin splitting exhibits the symmetry of a square, a rectangle, and a regular hexagon for the [001]-, [110]-, and [111]-grown quantum wells, respectively, as is demanded from the symmetry of the corresponding two-dimensional (2D) unit cells. For [110]-grown quantum wells an extreme anisotropy if found since the spin splitting is always zero for $\mathbf{k}_\parallel=(k_\parallel,0)$, i.e., [00$\bar{1}$].

In conclusion, we have numerically and analytically calculated the spin splitting of the conduction bands of GaAs/AlAs quantum wells grown along the [001], [110], and [111] directions. For large $\mathbf{k}_\parallel$, $k_\parallel \gg k_z^W$, the bulk result is essentially retrieved; the maximum spin splitting is cubic in $k_\parallel$ and approaches the maximum bulk value.

However, for small $\mathbf{k}_\parallel$, $k_\parallel \ll k_z^W$, different behavior is found: the spin splitting is linear in $k_\parallel$. This dependence does not originate from the well-known bulk linear k terms which are known to be very small.[4] It is caused by the confinement of the quantum-well states whereby k_z^W becomes quantized. We also note that in the linear regime the spin splitting averaged over all directions of $\mathbf{k}_\parallel$ is about a factor of 2 smaller for [110]-grown quantum wells than for [001]- and [111]-grown quantum wells. The magnitude of the spin splitting in the linear regime is 4 meV at $k_\parallel = 0.07(2\pi/a)$ for $\mathbf{k}_\parallel$ along [100] in a [001]-grown 25-Å GaAs/AlAs quantum well. The corresponding confinement energy $E_{\mathbf{k}_\parallel}$ is 580 meV. Larger values of the spin splitting, i.e., up to the bulk values ~ 50 meV, are obtained further out in the 2D Brillouin zone where cubic and bulklike behavior prevail. We note that the present theory does not accurately predict the spin splitting in this case since the bulk band structures of the constituents of the quantum well are not properly accounted for in the corresponding part of the 3D Brillouin zone.

It would be interesting to perform infrared spin-resonance or spin-polarized photoemission experiments on these systems to measure in particular the linear $k_\parallel$ dependence of the spin splitting for small $k_\parallel$. Thin quantum wells (~ 25 Å) should be used to obtain a maximum effect.

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