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Generalized effective-mass theory of subsurface scanning tunneling microscopy: Application to cleaved quantum dots

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An effective-mass theory of subsurface scanning tunneling microscopy (STM) is developed. Subsurface structures such as quantum dots embedded into a semiconductor slab are considered. States localized around subsurface structures match on to a tail that decays into the vacuum above the surface. It is shown that the lateral variation in this tail may be found from a surface envelope function provided that the effects of the slab surfaces and the subsurface structure decouple approximately. The surface envelope function is given by a weighted integral of a bulk envelope function that satisfies boundary conditions appropriate to the slab. The weight function decays into the slab inversely with distance and this slow decay explains the subsurface sensitivity of STM. These results enable STM images to be computed simply and economically from the bulk envelope function. The method is used to compute wave-function images of cleaved quantum dots and the computed images agree very well with experiment.

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I. INTRODUCTION

There is growing interest in the use of scanning tunneling microscopy (STM) to probe quantum states localized just under the surface of a semiconductor. For example, shallow donors in GaAs have been imaged recently^{1,2} as have Mn acceptors³ and the electronic states of cleaved self-assembled quantum dots.^{4,5} STM is able to probe these systems because it is a probe of the local density of states (LDOS) above the surface.⁶ The subsurface structure affects the LDOS hence can be probed by STM. But why does subsurface structure affect the surface LDOS so much that it can be imaged? And how can the images be simulated?

The puzzle is to understand how structure underneath the surface affects the LDOS above the surface. The surface modifies the quantum states of the semiconductor and embedded subsurface structures introduce further modifications. In many systems, including the experimentally important case of GaAs(110), the second-order effect that results from both modifications is likely to be small. Then the two effects decouple approximately and in the present work effective-mass theory is used to show that the lateral variation in the surface LDOS can be found from a surface envelope function. This is given by a weighted integral of the bulk envelope function that describes the localized states of the subsurface structure. This result explains the subsurface sensitivity of STM. In addition, it enables images to be computed simply and economically from known envelope functions.

To get more insight into the physics, consider a pure semiconductor with an ideal bulk-terminated surface. The bulk Bloch states match onto states that decay exponentially above the surface. The LDOS at energy E is the sum of the squared amplitudes of all Bloch states with energy E so the LDOS above the surface decays exponentially into the vacuum but is modulated in the lateral direction by the cell-

periodic parts of the Bloch functions. So the lateral variation in the LDOS is determined by the periodicity of the crystal lattice.

When subsurface structures such as quantum dots are introduced into a pure semiconductor of infinite extent, states occur in the band gap. These localized states decay exponentially in all directions but may be represented as a superposition of Bloch states. If this system is cleaved, the quantum states around each subsurface structure match onto a state that decays into the vacuum, however, the decay is no longer a pure exponential decay. Instead it is a superposition of exponential decays that reflects the superposition of Bloch states which forms the subsurface state. The LDOS is the squared amplitude of the superposition and it acquires a lateral variation whose length scale is determined by the width of the subsurface state.

The STM image of the subsurface structure is formed indirectly through its effect on the lateral variation in the LDOS above the surface. The only way to interpret the image is to understand the relation between the localized states of the subsurface structure and the LDOS above the surface. One approach is to calculate the LDOS with an atomistic method. However, the quantum states of typical subsurface structures are so broad that millions of atoms are needed to obtain accurate results. Atomistic calculations are difficult and expensive and offer little insight into the relation between the quantum states of the subsurface structure and the STM image.

Another approach is to use effective-mass theory. It gives an excellent description of shallow-impurity states, reproduces dot states semiquantitatively and gives a simple and intuitive picture of the physics of nanoscale semiconductor structures. But in its usual form, it cannot be used to find the surface LDOS. The problem is that the effective-mass wave function is a product of an envelope function and a band-edge Bloch function for the *bulk* material. This form does not

take account of the wave-function decay into the vacuum. It is clearly not valid in the *surface* region although it has been used to calculate images in some situations.⁷ A modified effective-mass theory that *can* be used to estimate the surface LDOS is the subject of the present work.

The main result is that the lateral variation in the LDOS above a subsurface structure can be described approximately by a surface envelope function. The integral that gives this function contains the product of the bulk envelope function of the localized quantum state of the subsurface structure and a slowly varying weighting function that is *independent* of the subsurface structure. So when the surface envelope approximation is valid, the lateral variation in the STM image can be found simply from the known bulk envelope function. In addition, the weight function has a power-law decay into the surface, in stark contrast to the exponential decay of localized states, including those in the STM tip. The slow decay generally explains why STM is sensitive to subsurface structure and images calculated with the present approach agree well with experimental data.

II. THEORY

A. Effective-mass theory

Effective-mass theory gives localized quantum states in a semiconductor in the form $\sum_m F_m(\mathbf{r}) U_m(\mathbf{r})$, where the functions U_m span the space of cell periodic functions and the Fourier expansion of each envelope function F_m is restricted to the first Brillouin zone.^{8,9} While the envelope function description is exact if all the terms are retained in the sum, it is most useful when the U_m are taken to be the periodic parts of the Bloch functions at a band extremum. In many cases, this allows the localized state to be approximated with a few envelope functions which are found from an effective-mass equation. In the simplest case of a shallow donor, only the conduction-band envelope function is needed.

The problem with applying this to the surface is that the wave function decays into the vacuum on an atomic length scale. This rapid decay cannot be described with envelope functions as the restricted Fourier expansion prevents each envelope function varying significantly on a length scale shorter than the unit cell. This means a large number of terms, $F_m U_m$, would be needed to make the envelope function description accurate. And there is another difficulty. The rapid variation in the potential at the surface means that the envelope functions would not obey simple effective-mass equations with a local potential. Instead, the generalized equations of Burt⁹ would have to be used but they involve a nonlocal potential that is difficult to deal with.

To see how to overcome these problems, consider a thick slab that consists of a stack of unit-cell layers. In a slab of pure material, without any subsurface structure, the potential is periodic in the two dimensions parallel to the surfaces. Deep inside the slab it is close to periodic in the third dimension but rises to zero in the surface regions. The potential barrier between the interior and the vacuum is a few electron volts so the quantum states decay exponentially into the vacuum on a length scale of a few angstroms. This system is termed the finite barrier slab (FBS). It can be idealized as a

system in which the potential rises to $+\infty$ at the surface with quantum states that go to zero at the surface and vanish in the vacuum. This system is termed the infinite barrier slab (IBS). In slabs such as GaAs (110), which have a mirror plane parallel to the surface, the IBS states are known to be a very good approximation to the FBS states.¹⁰ This important physics allows effective-mass theory to be generalized to find the surface LDOS.

The key step is to exploit the physics to neglect small quantities. Quantum states localized around a subsurface structure in a slab can be expressed as a superposition of slab Bloch states with coefficients that are determined from the Schrödinger equation. The surface LDOS can be found from the FBS coefficients, however, they are difficult to analyze. In contrast the IBS coefficients can be found easily. So consider what happens when the infinite barrier of an IBS is reduced to form an FBS. Clearly, both the coefficients and the Bloch states change. It turns out that whenever the second-order change from the Bloch states and coefficients is negligible, the effect of the subsurface structure decouples from the effect of the Bloch states. This allows the lateral variation in the surface LDOS to be found from a surface envelope function. Details are given in the next section.

B. Generalization to a slab containing subsurface structure

The FBS and IBS both consist of N unit cells of edge length d which occupy the region $0 \geq z \geq -L = -Nd$, where the sample thickness L is typically large. The FBS states decay exponentially to zero when $z > 0$ and $z < -L$ while the IBS states go to zero there. The IBS and FBS are periodic in the two dimensions parallel to the surfaces of the slab, $(x, y) \equiv \mathbf{p}$. Therefore the states as a function of $\mathbf{p}$ have Bloch form and can be labeled by a $\mathbf{k}$ vector parallel to the surfaces, $\mathbf{k}_{\parallel}$, a band index, n and an index, p to distinguish states within a band. Thus the IBS states are written as $\phi_{n\mathbf{k}_{\parallel}p}$ and the FBS states may be written as $\phi_{n\mathbf{k}_{\parallel}p} + \delta\phi_{n\mathbf{k}_{\parallel}p}$. When the unit cell has a mirror plane parallel to the surface the IBS states coincide with the truncated crystal states introduced by Zhang *et al.*¹⁰ These states are a good approximation to FBS (Ref. 10) and half-space ($z \leq 0$) slab¹¹ states in situations where coupling to surface states is weak. One system where this holds is GaAs (110),^{10,11} which is important because (110) is the natural cleavage plane of GaAs. When the truncated crystal states are a good approximation, $\delta\phi_{n\mathbf{k}_{\parallel}p}$ is expected to be small in the bulk and this is used to derive an approximate relation between states localized in the FBS and IBS.

The IBS and FBS states are complete so the localized states of an IBS containing a subsurface structure can be written as $\sum_{n\mathbf{k}_{\parallel}p} a_{n\mathbf{k}_{\parallel}p} \phi_{n\mathbf{k}_{\parallel}p}$. Similarly the FBS states are $\sum_{n\mathbf{k}_{\parallel}p} (a_{n\mathbf{k}_{\parallel}p} + \delta a_{n\mathbf{k}_{\parallel}p}) (\phi_{n\mathbf{k}_{\parallel}p} + \delta\phi_{n\mathbf{k}_{\parallel}p})$. When the localized state couples weakly to surface states, $\delta a_{n\mathbf{k}_{\parallel}p}$ is expected to be small and the FBS state above the surface is approximately $\sum_{n\mathbf{k}_{\parallel}p} a_{n\mathbf{k}_{\parallel}p} \delta\phi_{n\mathbf{k}_{\parallel}p}$ because $\phi_{n\mathbf{k}_{\parallel}p}$ is zero there. This approximation is a key step. All the effects of the localized state are contained in the coefficients $a_{n\mathbf{k}_{\parallel}p}$ which can be computed from IBS envelope functions without considering surfaces

while all the surface effects are contained in the functions $\delta\phi_{n\mathbf{k}_{\parallel}p}$ which can be found independently by calculating FBS states. Thus the difficulties of treating the surface may be avoided.

The IBS envelope functions, F_m , are used to find the $a_{n\mathbf{k}_{\parallel}p}$. The procedure is simple only when there is a mirror plane parallel to the surface and only this case, which includes GaAs(110), is considered here. In this case the IBS states are the odd parts of the Bloch functions of a periodic system of width $2L$: $e^{i\mathbf{k}_{\parallel}p}[e^{ik_{\perp}z}u_{n\mathbf{k}_{\parallel}k_{\perp}}(\mathbf{p}, z) - e^{-ik_{\perp}z}u_{n\mathbf{k}_{\parallel}k_{\perp}}(\mathbf{p}, -z)]$, where the $u_{n\mathbf{k}_{\parallel}k_{\perp}}$ are normalized to unity in $-L \leq z \leq L$ and $k_{\perp} = \pi p/L$, where p is an integer in the range 1 to N if band n is even under z inversion and 0 to N if it is odd. The envelope function expression, $\sum F_m U_m$, is found in the usual way^{8,9} with the unitary transformation $u_{n\mathbf{k}_{\parallel}k_{\perp}} = \sum_m \alpha_{n\mathbf{k}_{\parallel}pm} U_m$. Because of the mirror symmetry, the U_m are either odd or even under z inversion so the IBS states are

$$\sum_{m\mathbf{k}_{\parallel}p} \left[2b_{m\mathbf{k}_{\parallel}p} e^{i\mathbf{k}_{\parallel}p} \begin{pmatrix} \cos(\pi pz/L) \\ i \sin(\pi pz/L) \end{pmatrix} \right] U_m \equiv \sum_m F_m U_m,$$

where $b_{m\mathbf{k}_{\parallel}p} = \sum_n \alpha_{n\mathbf{k}_{\parallel}p} \alpha_{n\mathbf{k}_{\parallel}pm}$, the cosine factor applies when U_m is odd under z inversion and the sine factor applies when it is even. The F_m satisfy the effective-mass equations derived by Burt.⁹ The boundary conditions are $F_m \rightarrow 0$ at $z=0, -L$ when U_m is even and $\partial F_m / \partial z \rightarrow 0$ at $z=0, -L$ when U_m is odd.

When the F_m vary slowly, the FBS states above the surface can be approximated by the product of a surface envelope function and Bloch factor. Because the variation is slow, only small k Fourier components are significant so $u_{n\mathbf{k}_{\parallel}k_{\perp}} \sim u_{n00}$, $\alpha_{n\mathbf{k}_{\parallel}pm} \sim \delta_{nm}$, and $a_{n\mathbf{k}_{\parallel}p} \sim b_{n\mathbf{k}_{\parallel}p}$. In addition, $\delta\phi_{n\mathbf{k}_{\parallel}p}$ can be approximated. It has Bloch form, $\delta\phi_{n\mathbf{k}_{\parallel}p} = e^{i\mathbf{k}_{\parallel}p} w_{n\mathbf{k}_{\parallel}p}(\mathbf{p}, z)$ and if w varies slowly with $\mathbf{k}_{\parallel}$ and p , $w_{n\mathbf{k}_{\parallel}p} \sim w_{n00}$. In this case $\sum_{n\mathbf{k}_{\parallel}p} a_{n\mathbf{k}_{\parallel}p} \delta\phi_{n\mathbf{k}_{\parallel}p} \sim \sum_n (\sum_{\mathbf{k}_{\parallel}p} a_{n\mathbf{k}_{\parallel}p} e^{i\mathbf{k}_{\parallel}p}) w_{n00} \equiv \sum_n F_{sn}(\mathbf{p}) w_{n00}(\mathbf{p}, z)$, where F_{sn} is the surface envelope function. This form is similar to the one found in the theory of bulk shallow impurities⁸ and the approximations leading to it are also similar.

F_{sn} is found from F_n by using the approximation $a_{n\mathbf{k}_{\parallel}p} \sim b_{n\mathbf{k}_{\parallel}p}$ and performing the sum over $\mathbf{k}_{\parallel}$ and p . For an even band

$$F_{sn}(\mathbf{p}) = \frac{1}{iL} \sum_{p=1}^N \int_{-L}^0 F_n(\mathbf{p}, z) \sin \frac{\pi pz}{L} dz \equiv \int_{-L}^0 F_n(\mathbf{p}, z) G_n(z) dz, \quad (1)$$

where

$$G_n(z) = \frac{\sin(\pi z/2d) \sin[(N+1)\pi z/2L]}{iL \sin(\pi z/2L)}.$$

For an odd band, G_n is similar but $i \cos(\pi z/2d)$ replaces $\sin(\pi z/2d)$. The physics of subsurface STM follows from Eq. (1). The bulk envelope function for states localized around a subsurface structure is large in the subsurface region where $|z| \ll L$. In this regime $G_n \sim 2 \sin^2(\pi z/2d) / i\pi z$ so the influence of the subsurface state propagates to the surface with a weight $\sim 1/|z|$. This relatively slow decrease in weight

with depth is the reason why the surface LDOS is so sensitive to subsurface structure.

The validity of the surface envelope approximation depends mainly on the sensitivity of w to $\mathbf{k}_{\parallel}$ and p . This was tested with pseudopotential calculations performed with ABINIT.¹² Results for a GaAs slab within the central 10% of the Brillouin zone show that the w variation at 0.5 nm above the surface is $<12\%$ with the largest variation in the least significant Fourier components. This suggests that the approximation is accurate enough for qualitative and semiquantitative analysis of STM images.

Some modifications are needed to apply the theory to strained, heterogeneous systems such as cleaved self-assembled quantum dots. The cell periodic functions are defined in the way suggested by Burt⁹ and the effect of strain is taken into account with a coordinate transformation.¹³ When cleaved, a strained crystal relaxes so its surfaces are not flat. The coordinate transformation converts a strain relaxed slab into one with parallel faces and leads to a modified surface envelope function, $F_{sn} \rightarrow F_{sn}/\sqrt{J}$, where J is the Jacobean of the transformation. The effect of this is a few percent of the same order as the strain.

III. APPLICATION TO CLEAVED QUANTUM DOTS

To test the theory it is applied to the conduction-band states of a cleaved, self-assembled InGaAs cleaved quantum dot (CQD) embedded in a GaAs matrix. The conduction-band CQD states are found from a single-band approximation so the CQD state above the surface is approximately $F_{sc}(\mathbf{p}) w_{c00}(\mathbf{p}, z)$. However, as the atomic-scale structure due to $w_{c00}(\mathbf{p}, z)$ is not seen in the available experimental data only the large-scale variation caused by $F_{sc}(\mathbf{p})$ is compared with the experimental results.

A. Calculation

Excluding the atomic-scale factor, an approximation for the observed STM tunneling current I can be deduced from the results in Ref. 6. At tip position $(\mathbf{r}_t, z_t)$,

$$I = A \sum_j |F_{sc}^j(\mathbf{p}_t)|^2 f_t(E_j) g_t(E_j) T(E_j, eV), \quad (2)$$

where the j th eigenstate has energy E_j and surface envelope function F_{sc}^j and A is a constant that is treated as a fitting parameter. The tip density of states is $g_t, f_t(E_j) = 1/\{1 + \exp[(E_j - E_F)/k_B T]\}$ and E_F is the tip Fermi energy. The tunneling factor is

$$T(E_j, eV) = \exp(-2z_t \sqrt{2m\phi'/\hbar}),$$

where the average barrier height is $\phi' = (\phi_t - eV + \chi - E_j)/2$, $\phi_t = 4.5$ eV for the tungsten tip, and the electron affinity of GaAs is $\chi = 4.07$ eV. The relative contributions to I from each of the surface envelope functions can be controlled by varying E_F and this is done experimentally by altering the bias voltage on the tip. In the present case E_F is below the GaAs conduction-band edge and only the localized states of the CQD contribute significantly to the STM current.

FIG. 1. Plan (top) and cross section (bottom) of the CQD in the reference frame. The surface is at $z=0$. The growth direction is y with $y=0$ at the center of the dot and wetting layer system. The InAs fraction c varies linearly from 0.7 at the bottom of the dot to 1.0 at the top (Ref. 15).

The CQD envelope functions are calculated with a variation of the method in Ref. 14. The single-band, effective-mass Hamiltonian of the CQD is diagonalized exactly and, because only the blocks of the Hamiltonian with odd symmetry in z are included, the states go to 0 at the surface of the IBS where $z=0$.

The starting point for the calculation of the dot Hamiltonian is a model of the CQD (see Fig. 1) where the shape, size, and composition profile, $c(\mathbf{r})$, were determined by earlier topographic cross-sectional STM measurements.¹⁵ The dot Hamiltonian is

$$H = \frac{-\hbar^2}{2} \nabla M^{-1} \nabla + V(\mathbf{r}), \quad (3)$$

where M^{-1} is the strained effective-mass tensor and the electron confinement potential, $V(\mathbf{r}) = V_o(\mathbf{r}) + V_c(\mathbf{r})$, contains a contribution, $V_c(\mathbf{r})$, from the strain and a contribution, $V_o(\mathbf{r})$, from the position-dependent conduction-band offset.¹⁶ The strain field after cleaving the dot is calculated with a continuum finite element model and used to generate $V_c(\mathbf{r})$.¹⁷ The position-dependent components of the effective-mass tensor are then calculated from the strain field using first-order perturbation theory.¹⁷ Interestingly the electron confinement potential $V(\mathbf{r})$ is much deeper near to the interface than would be expected from the potential in an uncleaved dot and this is because, when cleaved, the dot relaxes and the strain is reduced.

To obtain rapid convergence (to within 0.1 meV) for the energies of the localized states the CQD eigenstates are expanded in a basis of one-dimensional (1D) harmonic oscillator functions¹⁴ with different length scales in each x , y , z direction. There are four states bound within the dot at energies of -226.0 , -120.5 , -57.1 , and -40.3 meV relative to the GaAs conduction-band edge. The dominant contribution to the in-gap STM current comes from only the two lowest energy states. These states are localized 4.2 nm and 3.8 nm, respectively, below the surface and the full width at half

maximum (FWHM) of their squared modulus is about 3 nm.

The tip-induced band bending seen in many STM experiments is not important here. The effect on the two lowest bound states of the CQD is small because their binding energy is large. This was confirmed by using a 1D model to compute the effect of tip-induced band bending at a tip voltage of 1 V (near the center of the experimental range). This additional potential pushes the states away from the surface and this reduces the amplitude and the width of the surface envelope functions. But the amplitude of these functions is unimportant and the FWHM of the two lowest energy functions changes by only 4.7% and 0.4%, respectively. For simplicity, the tip-induced band bending is therefore neglected.

Image charge effects are also small and have been neglected. The abrupt dielectric interface between the dot and vacuum at the cleavage plane introduces an image potential. Our calculations suggest the effect of this potential is small, of the order of 5 meV on the dot binding energies and less than 0.5% on the FWHM of the two lowest surface envelope functions.

B. Experiment

Cross-sectional scanning tunneling spectroscopy experiments were performed under UHV conditions ($P < 4 \times 10^{-11}$ Torr) using an omicron STM1, TS-2 scanner, with tips prepared as described in Ref. 18. The measurements were performed on *in situ* cleaved (110) surfaces of molecular beam epitaxial structures containing InGaAs dots within a GaAs matrix. The details of the sample preparation have been reported elsewhere.¹⁵ To investigate the CQD electronic structure, current imaging tunneling spectroscopy was acquired simultaneously at room temperature with the topographic images shown in Ref. 15. At every point on a 0.09×0.09 nm² grid, tunneling spectroscopy (I - V) curves were measured at every 0.015 V between bias voltages of -2.6 and 2 V with the feedback loop switched off. The vertical position of the tip was therefore held stationary and all topographical dependencies on the tunneling current were removed. Tunneling below the GaAs band gap, into the empty CQD states, was observed between 0.7 and 1.2 V. At higher voltages a significant amount of tunneling into the GaAs matrix was observed in addition to the tunneling into the dot states. To reduce the noise in each data set, each spatial point was averaged over six consecutive voltage points.

C. Comparison between theory and experiment

Figure 2 shows experimental and calculated in-gap STM currents along a line in the x direction through the center of the CQD at $y=0$ nm. The comparison between experiment and theory is restricted to low-bias voltages (0.7–1.2 V) where the tunneling is predominantly into the lowest bound states in the CQD. As the voltage range is small, the tip Fermi energy can be assumed to vary linearly with applied voltage, $E_F = \alpha V + \beta$, where α and β are constants. The actual relation between E_F and V is unclear because of the tip-induced band bending and hence α , and β [in addition to the constant A in Eq. (2)] are treated as fitting parameters and adjusted to give the best match between the calculated in-gap

FIG. 2. In-gap STM current along x at $y=0$ nm. Dashed lines: experiment. Solid lines: calculation. The four pairs of curves are at different V (E_F). Each successive pair of curves is offset by 2 pA. Bottom: $V=0.72\text{--}0.81$ V ($E_F=-226$ meV), second: $0.83\text{--}0.92$ V ($E_F=-181$ meV), third: $0.94\text{--}1.03$ V ($E_F=-136$ meV), and top: $1.05\text{--}1.14$ V ($E_F=-91$ meV). E_F is given relative to the GaAs conduction-band edge.

STM current and the experimental data. In Eq. (2), $T(E_j, eV)$ was approximated by the WKB result for a square barrier between the tip and the quantum dot. However, the exact form of T has little effect on our calculated results: at $E_F=-91$ meV, approximating $T(E_j, eV)$ by unity results in a change in the FWHM of I of less than 2%.

To obtain the curves in Fig. 2 the values $\alpha=410\pm 90$, $\beta=-540\pm 70$ meV, and $A=1.8\pm 0.3\times 10^5$ are used. At the lowest bias voltage, where the tunneling is only into the ground state, the experiment and theory fit extremely well. At higher voltages the fit is still reasonable although the calculated curves are slightly too narrow. At large V the tip-induced band bending might be expected to be important but this will reduce the width of the calculated curves. Instead, the difference between experiment and the calculation is more likely to be caused by alloying between dot and matrix material at the dot edges which will soften the edges of the confinement potential and increase the width of the more weakly bound states.

IV. CONCLUSION

A simple technique for calculating quantum states above subsurface structures has been developed. The approach relies on two approximations. First, the quantum state of the substructure is found from the bulk envelope function for the structure in an infinite barrier slab and the band states of a finite barrier slab. Then a second approximation is used to express the state above the surface as the product of a surface envelope function and a Bloch factor. The slow variation in the weight factor used to calculate the surface envelope function from the bulk envelope function explains the subsurface sensitivity of STM and computed wave function images of a cleaved self-assembled dot are in good agreement with experiment.

The approach developed here applies to any subsurface structure, provided the approximations leading to the surface envelope function are valid. In addition, it is most convenient when a single-band approximation is valid. The results in Sec. III C suggest that this is the case for cleaved quantum dots. Currently, there is also significant interest in STM imaging of subsurface impurities but the physics of impurities very close to the surface is not well understood. There is evidence that the effective-mass approach with a small number of bands loses accuracy when the impurities are very close to the surface^{1,19} and tip-induced band bending can change the occupancy of impurity states and modify the STM image.^{1,2} Further analysis is therefore needed to determine whether the quantum states of near-surface impurities satisfy the conditions needed to apply the present approach. In all cases, the approximations developed here are likely to be most useful for computing the large-scale structure of wave-function images, rather than atomic detail. They have the advantages that images can be computed easily from known envelope functions and at a much lower computational cost than atomistic calculations.

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