Quantum confinement in nanocorrugated semiconductor films

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Numerical simulations were performed to predict the electron energy levels and wave functions in periodically nanocorrugated free-standing InAs films. The obtained data show that in films thinner than 4 nm the lowest energy levels are due to the *X*-conduction-band valleys. In such films, the elastic strain gives rise to a periodic potential consisting of quantum wells about 1 eV deep, resulting from the strain-induced shift of the energy position of the *X*-valley minimum. The possibility of localization of electron states in the potential wells is shown.

The present-day semiconductor technology is rapidly progressing toward the fabrication of nanoscale devices. Recently, a nanostructuring method was introduced, enabling the fabrication of various semiconductor nanoshells from strained pseudomorphic heterofilms detached from substrates on which these heterofilms were initially grown.[1,2] In fabrication of the nanoshells, A_3B_5 semiconductor[1,2] and Si/SiGe (Refs. 2 and 3) were used. This method is based on the tendency, displayed by detached films, to assume a shape providing for the minimum possible elastic energy in the final structure; as a result, the films roll in tubes[1] or undergo buckling to form corrugated structures.[2] The proposed method allows one to obtain shells of various complex shapes with nonuniform distribution of strains in them.[3] A unique property of such 3D shells is sharp variation of the strain over nanosizes. For instance, the strain ε can vary along the film by several percent, resulting in considerable band-edge shifts of $\Delta E_c \sim a_c \varepsilon \sim 0.5$ eV, where a_c is the deformation potential, forming potential wells and barriers at the nanometer scale and leading to quantum confinement. The local detachment of a film from the substrate itself gives rise to a potential well.

The purpose of the present study was to calculate the energy spectrum and wave functions of electrons in a periodically nanocorrugated thin-film structure of fundamental and practical interest.[2] An example of such a structure with four spatial periods is schematically depicted in Fig. 1; the number of the periods can be made infinitely large using longer strips detached from the substrate. (The detachment is achieved by selective removal of the substrate or a sacrificial layer at the edge of the structure[2]). The flat state of the released film is unstable, and the film buckles to form a corrugated shell. In this way or another, the elastic stress in the released film relaxes, lowering the conduction-band edge and forming a potential well for electrons.

In this nanostructuring method, single- or multi-layered compressed films to be freed from substrates can be used. The role of corrugation is most readily illustrated with the case of a bifilm that comprises a conducting layer [the upper layer in Fig. 2(a)] and an underlying insulating layer. Apparently, the conducting layer is tensile stressed and compressed, respectively, in regions 1 and 2 of the film. With a small bending radius, an ultimately high strain can be achieved, which causes the band edges to shift appreciably,

the band edges in regions 1 and 2 shifting in opposite directions. Thus, in the nanometer region the corrugated system presents a space-periodic sequence of potential wells of rather large depth.

The prediction of electronic levels in the nanocorrugated structure can be reduced to solving the following problems: (i) determination of the potential relief for electrons in the elastically deformed nanostructure and (ii) solution of the Schrödinger equation for electrons in the obtained potential.

In the present study, these calculations were performed under the following simplifying assumptions:

1. The strains in the thin films ($d \sim 1$ nm) were allowed for in the framework of the continuum elasticity theory. This assumption is justified by a comparison of strains in thin films predicted in the atomic-elasticity approximation and in the approximation of the continuum elasticity theory; the comparison shows that the elastic theory can be used to predict strains even in very thin GaAs films [down to 2 MLs (0.56 nm)].[4] In addition, the experiment shows[1] that the radius of nanotubes rolled up from free heterolayers can be adequately predicted by a formula obtained in the continuum theory[5] for layers as thin as 4 MLs (1.1 nm).

2. The Schrödinger equation for electrons in the corrugated structure was solved in the effective mass approxima-
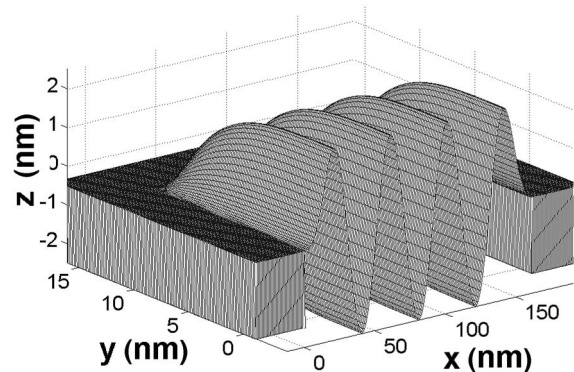

FIG. 1. Schematic view of the nanocorrugated structure. Only the shape of the corrugated film is illustrated. The *x*-*z* cross section of the film is shown in Fig. 2(a). The substrate is oriented normally to the (001) direction. Note the difference between the scales along the different axes.
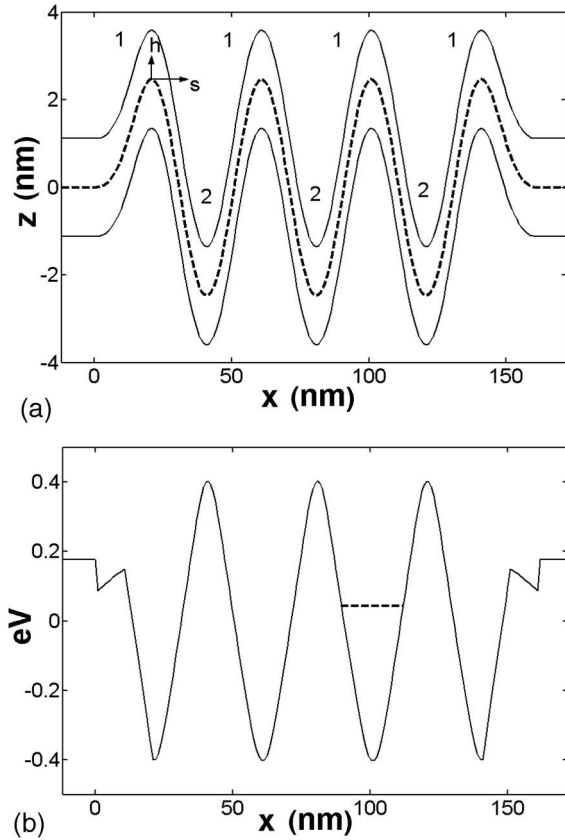
FIG. 2. (a) x-z cross section of the structure from Fig. 1. The middle surface is shown with a dotted line. Axes s, h used in the calculation are also shown. Regions 1 are under tensile strain and regions 2 are under compressive strain. (b) Confinement potential for electron near the upper surface of the film (solid line) and lower electron level (dotted) line.

tion. In thin films, the translation symmetry across the film is lacking; yet, the calculations performed by the pseudopotential method[6] and by the empirical tight-binding method[7] yield the position of electronic levels in GaAs films with thickness down to 2–3 ML (0.7–0.8 nm), which very closely coincides with that of the levels predicted by the effective mass approximation. The films in which the difference is large ($d < 1$ nm) are not considered here.

To determine the shape of a freed film and predict the strains in it, one has to solve the problem of the theory of elasticity for shells,[8] which in the case of a heavily deformed body reduces to the solution of complex nonlinear Föpple–von Kármán differential equations. The latter equations can be solved analytically only in several particular cases.[9]

It is known from the experiments with nanocorrugated structures[2] and from the theory of elasticity for macrocorrugated structures[10] that the shape of the structures is close to a sinusoid. The amplitude of the sinusoid is easy to estimate. We assume that the elastic stress has already dropped to a value such that inside the film [Fig. 2(a)] there is a neutral surface where strains are zero. The length of the fully relaxed film, measured along the neutral interface, is $L(1+\Delta f)$. This length geometrically defines the corrugation amplitude (here, L is the length of the compressed film and Δf is the lattice

mismatch in the structure). As it is seen from Fig. 2, the amplitude of the corrugation is large, amounting to about 2.4 nm. The chosen corrugation parameters fall into the range of experimentally obtained values.[2]

With the known shape of the structure, following the work[11] and led by simple geometric considerations, we can calculate the strain distribution in the structure. We introduce a curvilinear coordinate system chosen with due regard for the geometry of the structure [Fig. 2(a)]. The coordinates s and h are directed along the surface of the film and along the normal to it, and the point $h=0$ is chosen at the middle of the film. Nothing prevents the film from being deflected in the y direction (Fig. 1) excluding for the region immediately adjacent to the undetached part of the film; we therefore assume the strain ε_y in this direction to be zero. It is well known[5,8] that the strain ε_s in a film in the direction along the surface varies linearly across the film: $\varepsilon_s=h/R$, where h is the thickness of the film and R is its curvature radius calculated by the differential-geometry formulas. This strain may be rather high. In the structure depicted in Fig. 1, the lattice mismatch between the film and the substrate is $\Delta f=3\%$, and the corrugation period is $b=40$ nm. The minimum curvature radius for this structure is $R_{min}=16$ nm. For the film thickness of $d=8$ ML (2.2 nm), the strain ε_s amounts to 7%. The strain ε_h in the h direction can be predicted using the Poisson relation $\varepsilon_h=-[\nu/(1-\nu)]\varepsilon_s$, where ν is the Poisson ratio.

The strain distribution thus obtained makes it possible to calculate the potential relief in the nanocorrugated structure. Note that the relief for electrons in the Γ valley will differ from that for electrons in the X valleys because the band edges in these valleys shift by different values.[12] As the film thickness gradually decreases, the energy level in the X valley will become the lowest quantum level because the effective mass in this valley is greater and the rise of the quantization levels in it is less pronounced than in the Γ valley.[13] In free GaAs films, the change of the succession of the valleys occurs at the thickness of 8 MLs (2.2 nm).[14] Estimations show that in InAs films thinner than 12 MLs (3.3 nm), where the energy gap between the Γ and X valleys amounts to 1 eV,[15] the lowest level is the X valley electron level.

In strain-free InAs, the X-conduction-band valley is known to be sixfold degenerate. In this valley, the constant-energy surfaces are ellipsoids characterized by a heavy longitudinal mass $m_l=1.13m_0$ and light transverse mass $m_t=0.16m_0$,[15] where m_0 is the free-electron mass. In the film under consideration, grown on a (001) substrate, there are two X_z valleys oriented across the film and four in-plane oriented X_{xy} valleys. In the strained film, the strain-induced shifts of the energy minima in the X_z and X_{xy} valleys are $\Delta E_c^z=a_c(\varepsilon_s+\varepsilon_h+\varepsilon_y)+\frac{2}{3}\Xi_u(\varepsilon_h-[(\varepsilon_s+\varepsilon_y)/2])$ and $\Delta E_c^{xy}=a_c(\varepsilon_s+\varepsilon_h+\varepsilon_y)-\frac{1}{3}\Xi_u(\varepsilon_h-[(\varepsilon_s+\varepsilon_y)/2])$, respectively,[12] where a_c is the deformation potential for electrons, and Ξ_u is the shear deformation potential. The first, hydrostatic, term shifts both types of valleys by the same energy, whereas the second, shear, term causes an energy splitting of the two types of valleys. In the structure of interest, the upper film at points 1 [see Fig. 2(a)] is in tension; here, $\varepsilon_s > 0$, $\varepsilon_y=0$ and $\varepsilon_h < 0$ and, hence, the X_z valleys lie approximately 0.5 eV above the X_{xy} valleys. The situation at points 2 is opposite;

yet, the hydrostatic strain at these points raises the both types of valleys to a higher-energy position compared to points 1 [Fig. 2(a)]. Moreover, the quantization because of the transverse electron confinement in the X_z valleys is defined by the larger longitudinal mass m_l compared to the X_{xy} valleys, where the quantization due to confinement in the film-normal direction is determined by the small transverse mass m_t. Thus, the lowest energy levels in our structure are the levels due to the X_z valleys. Direct calculations confirm this conclusion. In what follows, we consider only the energy levels for electrons in the X_z valleys.

With the above expressions for the strains taken into account, the shift of the X_z-valley edge in the structure of interest is $\Delta E_c^z = \left[a_c(1-2\nu)/(1-\nu) - \frac{1}{3}\Xi_u(1+\nu)/(1-\nu) \right] h/R$. This shift varies linearly across the film, the slope of the strain-coordinate dependence being determined by the curvature radius of the film. Figure 2(b) shows this dependence near the upper surface of the film. The values of parameters used for InAs were as follows: $a_c = -6.08$ eV (Ref. 15) and $\Xi_u = 4.5$ eV.[12] The film was assumed to consist of two layers of identical thicknesses, a top InAs layer and a narrow layer grown from a high energy-gap semiconductor or a dielectric, with a 2 eV barrier at the heterointerface between the layers. In the calculations, the film-vacuum interface was assumed to act as an infinitely high barrier for electrons. At the interface between the detached from the substrate and the undetached parts of the film there is a 0.2 eV barrier for electrons.

The potential relief obtained defines the position of energy levels and the wave functions of electrons in the nanocorrugated structure. We solve the Schrödinger equation in the cross section of the structure [Fig. 2(a)]. This approximation is well justified since the shape of the structure in the y direction remains almost unchanged over a substantial distance [2,10] (Fig. 1), and the shape of the potential well along the y direction is close to a rectangle. The use of the two-dimensional approximation for the Schrödinger equation implies that we take into account only the lowest quantum state with respect to the energy of the electron motion along this direction. In the effective mass approximation, the Schrödinger equation in the chosen curvilinear coordinate system is[16]

$$-\frac{\hbar^2}{2}\left[\frac{1}{m_h^*}\frac{1}{H_s}\frac{\partial}{\partial h}\left(H_s\frac{\partial\psi}{\partial h} \right) + \frac{1}{m_s^*}\frac{1}{H_s}\frac{\partial}{\partial s}\left(\frac{1}{H_s}\frac{\partial\psi}{\partial s} \right) \right] + U(s,h)\psi$$
$$= E\psi,$$

where $H_s = 1 + h/R(s)$, U is the potential energy, E is the electron level, and ψ is the electron wave function. The first term in the Schrödinger equation is the kinetic-energy operator written in the curvilinear coordinates with due allowance for the effective-mass anisotropy in the X_z valleys. In the case under consideration, the mass in the h direction is equal to the longitudinal mass: $m_h = m_l$, and the mass in the s direction, to the transverse mass: $m_s = m_t$. The potential energy takes into account the strain-induced shift of band edges and the band discontinuity at the heterointerface. The Schrödinger equation was transformed into a finite-difference equation on a rectangular calculation grid in the coordinates (s, h), whose solution was reduced to the solu-
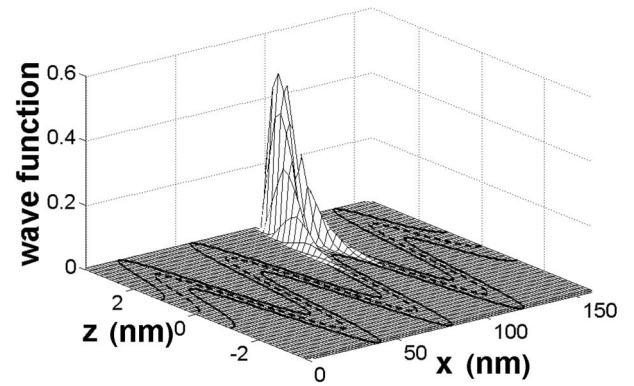

FIG. 3. The wave function of one of the lowest electron states. Other states with the same energy are localized in other potential wells that arise in the tensile-stressed regions of the upper film [regions 1 in Fig. 2(a)]. The total number of the degenerate states is defined by the number of the corrugation periods along the x axis.

tion of an eigenvalue problem for the obtained system of linear equations.

The numerical solution of the Schrödinger equation showed that the lower electronic state lies at an energy of 0.45 eV over the bottom of the potential well [Fig. 2(b)]. With the chosen parameters of the structure, there is no significant tunneling-induced coupling between the potential wells. The lower electronic states are essentially degenerate, and the wave functions of electrons in this state can be taken as localized in individual potential wells (Fig. 3). Meanwhile, there is Coulombic interaction between the electrons in individual wells, and such a nanostructure as a whole can be considered as a kind of a quantum dot molecule.

Corrugated structures can also be fabricated from single-layered films. In the latter case, the corrugation gives rise to tunneling coupled potential wells in all regions of the structure adjacent to the convex surface of the film [Fig. 2(a)]. The numerical solution of the Schrödinger equation showed that the wave function of the lowest state is delocalized, being distributed among the different wells: the maxima of the wave function coincide with the potential-energy minima. Such a nanostructure can be regarded as a quantum dot whose bottom has a spatially modulated potential relief.

The calculations were performed under the assumption that the elastic stress in the freed part of the film has dropped to a value so small that inside the film there is a neutral interface. This assumption may not be valid;[10] in this case, a compressive strain will remain everywhere inside the film. This strain adds to the above-considered strain to give rise to some rise of the conduction-band edge over the entire structure. Yet, as our calculations show, the final results in this case will remain qualitatively unchanged even with the residual compression equal to half the initial compression.

The effective mass approximation as applied to calculation of the energy levels may appear violated for thin films; in such cases an electrons in a film should be treated as a free electron in a quantum well rather than an electron in a semiconductor.[6,17] Our calculations carried out under the assumption that the electron mass is equal to the free-electron

mass yielded a stronger localization of electron states. To summarize, the above-considered nanocorrugated structure presents a thin-film quantum system with an energy spectrum defined by the strains present in the structure.

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