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DENSITY OF CONFINED STATES IN FINITE-BARRIER QUANTUM WELLS

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Density of states (DOS) is one of the most important characteristics of quantum-well materials, significantly impacting their electronic and optical properties. For example, gain characteristics and lasing threshold of quantum-well semiconductor lasers are largely dependent upon the DOS. Yet, surprisingly little attention has been paid to the effects of finite-barrier height on the DOS in quantum wells. In spite of its weak foundation, the standard approach[1] is to use an expression derived in a strictly two-dimensional (2D) case which for quantum wells with infinitely high barriers has been shown[2] to correspond with the bulk density of states. In an attempt to account for a more realistic case of finite-height potential barriers, a modified 2D DOS with the effective mass averaged between the well and the barrier materials was used occasionally[3]. In this paper, we propose a new expression for the DOS in finite-barrier quantum wells based on the correspondence principle and on rigorous calculations of the quantized wave vectors.

In the infinite-barrier limit, the 2D DOS is known to coincide with the bulk case at the bottom of each subband[2]. This "conservation of states" is no longer satisfied for finite-barrier quantum wells, regardless whether the standard expression (Ref. 1) or an average effective mass with the confinement probability as the weighting factor (Ref. 3), is used. In addition, both previous expressions for the quantum-well DOS per unit volume give unphysically high values when the confined-state energy reaches the top of the well. Hence, in addition to introduction of the average effective mass for finite-barrier quantum wells, we propose calculation a the density of states over an effective volume such that the cumulative quantum-well density of states satisfies again the correspondence with the bulk case.

Our approach is based on the fact that while the in-plane area of the quantum well is well defined, it is not clear what should be the volume over which the DOS per unit volume should be calculated. The reason for this difficulty is penetration of the electronic wave function into the barrier regions. Hence, the correspondence with the bulk DOS is used as a guideline to determine for each subband n the corresponding effective well width $L_{eff,n}$ that enters into the finite-barrier quantum well DOS.

In order to illustrate the significance of the new definition of the DOS, we consider symmetric rectangular conduction-band quantum wells in the $GaAs/Al_{0.3}Ga_{0.7}As$ material system at room temperature (300 K). Fig. 1 shows the variation of $L_{eff,n}$ with the quantum well width L_z for five lowest subbands. For large values of L_z, when the quantum well displays essentially bulk behavior, it is expected that $L_{eff,n}$ should approach L_z. Therefore, it may seem somewhat surprising that even at 50 nm there is a significant difference (~6%) between $L_{eff,n}$ and L_z. This is caused by the fact that even at such large values of L_z, the solutions of the eigenvalue equation for the propagation constant $k_{z,n}$ in a finite-barrier quantum well are still significantly different from the infinite-barrier case. In fact, there is still a 1% difference between these solutions even at L_z as large as 200 nm. On the other hand, when L_z becomes sufficiently small for the energy level n to approach the top of the well, the electronic wave functions extend substantially into the barrier region, resulting in an increased value of $L_{eff,n}$. Consequently, $L_{eff,n}$ reaches a minimum at a certain value of L_z.

Fig. 2 shows the conduction-band DOS in finite-barrier QWs calculated using the strictly 2D formula (Ref. 1), the same formula but with an average effective mass (Ref. 3), and the approach described in this work. It is clear that significant departure from the conventional DOS arise when the electronic wave function associated with a given subband state penetrates significantly into the barrier regions. As shown in Fig. 2, we expect that irrespective of the subband index, at the top of the well the density of confined states reaches the same maximum value of ~0.063 $nm^{-3}eV^{-1}$.

In many applications that do not involve a very high carrier density, occupation of the first subband is the only one that needs to be considered. It is remarkable that the most dramatic reduction of the density of confined states, compared to conventional expressions, is obtained for the lowest subband, especially for thin quantum wells with L_z < 5 nm.

The results presented in this paper, obtained by applying the correspondence with the bulk DOS, indicate that the DOS in finite-barrier quantum wells differs substantially from the conventional 2D DOS calculated for infinite-barrier quantum wells.

References

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2. M. W. Prairie and R. M. Kolbas, Superlattices & Microstructures 7, 269 (1990).
3. G. Bastard and J. A. Brum, IEEE J. Quantum Electron. QE-22, 1625 (1986); S. Wang, *Fundamentals of Semiconductor Theory and Device Physics*, Prentice Hall, Englewood Cliffs 1989, p. 556.

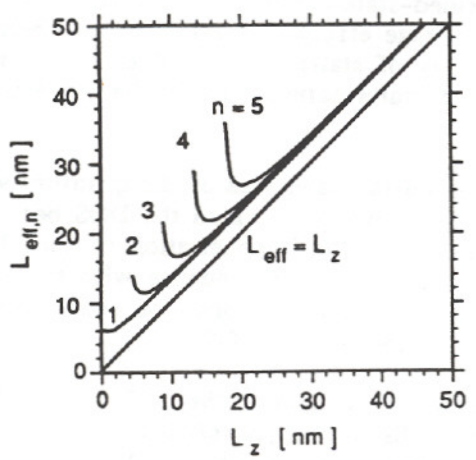

Fig. 1. Effective width of the quantum well $L_{eff,n}$, as defined in text, for subsubband n in the conduction band of rectangular $GaAs/Al_{0.3}Ga_{0.7}As$ quantum wells. The line $L_{eff} = L_z$ is added to help guide the eye.

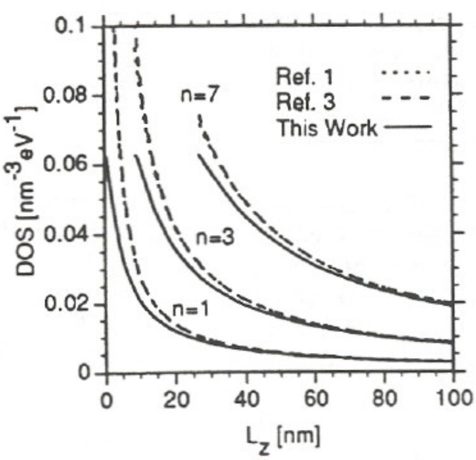

Fig. 2. Comparison of the conduction-band DOS at the bottom of subbands 1, 3, and 7 in $GaAs/Al_{0.3}Ga_{0.7}As$ rectangular quantum wells, as calculated in this work, with the results obtained using previous approaches. Note sig nificant differences for the lowest subband in narrow quantum wells.