

Mobility enhancement in quantum wells by electronic-state modulation

Takuma Tsuchiya

Fujitsu Laboratories Ltd., 10-1 Morinosato-Wakamiya, Atsugi 243-01, Japan

Tsuneya Ando

Institute for Solid State Physics, University of Tokyo, 7-22-1 Roppongi, Minato-ku, Tokyo 106, Japan

(Received 29 December 1992)

A wave-function modulation induced by insertion of several thin barrier layers inside a quantum well is proposed as a method of enhancement of the electron mobility limited by scattering from optical phonons. Numerical calculations demonstrate appreciable enhancement for appropriate values of the parameters for which intersubband scattering processes are suppressed.

I. INTRODUCTION

Realization of high electron mobility is one of the most challenging subjects in semiconductor physics and is important for device applications. The modulation doping technique is one of the most successful examples that have worked well at low temperatures.¹ In this paper, we propose a method to increase the electron mobility limited by optical-phonon scattering in quantum wells by a modulation of wave functions along the direction perpendicular to the layers and demonstrate the mobility enhancement by a numerical calculation.

In modulation doped heterostructures, polar-optical-phonon scattering is the most important mechanism that limits electron mobility at room temperature. Optical phonons in heterostructures can be strongly modified by the presence of heterointerfaces as has already been discussed in many review articles.²⁻⁸ This has led to the expectation that optical-phonon scattering is reduced and a high room-temperature mobility is realized in quantum wells and superlattices. In fact, numerous calculations of scattering strength have been reported so far.⁹⁻²⁸ In these calculations various models of optical phonons were used and some^{21,25} actually predicted a reduction of the scattering rate with decreasing well thickness. Recent more reliable calculations based on lattice displacements obtained in lattice-dynamical calculations have given a disappointing result that the scattering strength is essentially independent of such phonon modulation due to the presence of heterointerfaces.²⁹⁻³²

It is now well established that the scattering strength decreases with increasing layer thickness in GaAs/AlAs quantum wells as long as contributions from intersubband scattering are negligible. This is due to a change in the form factor for the interaction with phonons determined by the electron wave function along the direction perpendicular to the layer and suggests that the scattering strength is more sensitive to the electron wave function than the phonon modulation. The long-range Coulombic nature of interaction with optical phonons suggests another possible way of reducing the scattering strength through a modulation of the electron wave function.

In this paper, we calculate the electron mobility of GaAs/AlAs quantum wells with several thin barrier layers being inserted and show that the scattering strength can be reduced due to a wave-function modulation induced by such thin barrier layers. Because phonon modulation due to the presence of heterointerfaces affects the scattering strength only very weakly, we shall employ a bulk-phonon model in which optical phonons in bulk material constituting the well layer are assumed. The model and the method of calculating the electron mobility are discussed briefly in Sec. II, the result is presented in Sec. III, and a short summary is given in Sec. IV.

II. SCATTERING FROM OPTICAL PHONONS

We consider the following two structures consisting of GaAs and AlAs: One is a conventional single quantum well and the other is a single quantum well with thin AlAs barrier layers being inserted. The former will be denoted as SQW and the latter as wave-function-modulated SQW or WFMSQW. Figure 1 shows the band diagram of these systems and the wave function of the

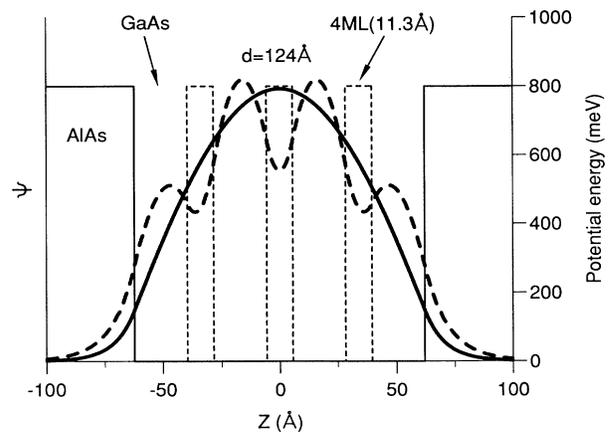


FIG. 1. Band diagram and wave function of the lowest subband of SQW (solid line) and WFMSQW (dashed line) with layer thickness 124 Å.

ground subband for the total layer thickness $d=124$ Å. The height of all barriers is 800 meV. Three thin barriers with thickness 11.3 Å corresponding to four monolayers of AlAs are inserted in equal spacing. These barriers modulate the electron wave function in such a way that it has an appreciable amount of short-wavelength components. Note that this structure is similar to that used recently in the experiments by Zhu *et al.*³³

The presence of such barrier layers tends to raise the energy of subbands whose wave function does not have a node at the position of the barrier. This leads to a bunching of several subbands into groups. In the presence of three equally spaced barriers, for example, four adjacent subbands tend to have energies close to each other. Consequently, the introduction of barrier layers gives rise to extra intersubband scattering in addition to the desired wave-function modulation. Thus, explicit numerical calculations are required to see whether such a wave-function modulation can really enhance the mobility.

Because optical-phonon scattering is dominant above 77 K, other scattering mechanisms such as impurities and acoustic phonons are completely ignored. The effective-mass approximation is employed for electronic states and the difference in the effective mass of well and barrier layers is neglected. Furthermore, we consider the case of low electron concentration ($N_s=2\times 10^{11}$ cm⁻²) for which band bending is not important. We shall neglect the screening effect because of high phonon frequency ($\gtrsim 36$ meV), low electron concentration, and high temperatures.

We employ a bulk-phonon model for optical phonons. It has been shown in previous papers³⁰⁻³² that the com-

pleteness of phonon modes leads to the conclusion that the scattering rate does not depend on details of individual phonon modes. In fact, the scattering strength is determined essentially by spatial distribution of the product of the Fröhlich constant α , LO-phonon frequency $\hbar\omega_{\text{LO}}$, and the average phonon number $n(\hbar\omega_{\text{LO}})$.²⁴ When a part of GaAs is replaced with AlAs, therefore, we can roughly estimate the change of the scattering rate by subtracting the contribution of the GaAs at the part and add that of AlAs there. In Table I, we summarize α , $\hbar\omega_{\text{LO}}$, $n(\hbar\omega_{\text{LO}})$, and the polaron damping rate $\Gamma (= \alpha\hbar\omega_{\text{LO}}n)$ at 300 and 120 K for GaAs and AlAs LO phonons. The electron effective mass is chosen as that in GaAs for both cases. It is found that Γ in AlAs at 300 K is almost the same as that in GaAs. Thus, the bulk-phonon model is quite accurate for GaAs/AlAs systems at 300 K and may slightly overestimate the scattering strength at 120 K.

The electron mobility will be calculated in the relaxation-time approximation. We have

$$\mu = \frac{e\langle\tau\rangle}{m_e}, \quad (2.1)$$

with $-e$ being the electronic charge and m_e the effective mass ($m_e=0.067m_0$, m_0 being the free-electron mass). The momentum relaxation time $\langle\tau\rangle$ is given by the average over different subbands,

$$\langle\tau\rangle = \frac{\sum_l \langle\tau_l\rangle N_l}{\sum_l N_l}, \quad (2.2)$$

where $\langle\tau_l\rangle$ and N_l are the relaxation time and the electron sheet density of the subband l . We have

$$\langle\tau_l\rangle = \frac{\sum_{k_{\parallel}} [E_l(k_{\parallel}) - E_l(0)] \tau_l [E_l(k_{\parallel})] (-df/dE)|_{E=E_l(k_{\parallel})}}{\sum_{k_{\parallel}} [E_l(k_{\parallel}) - E_l(0)] (-df/dE)|_{E=E_l(k_{\parallel})}}, \quad (2.3)$$

where $f(E)$ is the Fermi distribution function. The relaxation time for state $(\mathbf{k}_{\parallel}, l)$ with energy $E_l(k_{\parallel})$ is given by

$$\begin{aligned} \frac{1}{\tau_l [E_l(k_{\parallel})]} &= \frac{2\pi}{\hbar} \sum_{l'} \sum_{\mathbf{q}} |M(\mathbf{k}_{\parallel}, l; \mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}, l'; q_z)|^2 \left[\frac{1 - f[E_{l'}(|\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}|)]}{1 - f[E_l(k_{\parallel})]} \right] \delta[E_l(k_{\parallel}) - E_{l'}(|\mathbf{k} + \mathbf{q}_{\parallel}|) + \hbar\omega_{\text{LO}}] \\ &\quad \times \left[1 - \frac{|\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}|}{k_{\parallel}} \cos\theta(\mathbf{k}_{\parallel}, \mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}) \right] n(\hbar\omega_{\text{LO}}) \\ &+ \frac{2\pi}{\hbar} \sum_{l'} \sum_{\mathbf{q}} |M(\mathbf{k}_{\parallel}, l; \mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}, l'; q_z)|^2 \left[\frac{1 - f[E_{l'}(|\mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}|)]}{1 - f[E_l(k_{\parallel})]} \right] \delta[E_l(k_{\parallel}) - E_{l'}(|\mathbf{k} - \mathbf{q}_{\parallel}|) - \hbar\omega_{\text{LO}}] \\ &\quad \times \left[1 - \frac{|\mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}|}{k_{\parallel}} \cos\theta(\mathbf{k}_{\parallel}, \mathbf{k}_{\parallel} - \mathbf{q}_{\parallel}) \right] [n(\hbar\omega_{\text{LO}}) + 1], \end{aligned} \quad (2.4)$$

TABLE I. Fröhlich coupling constant α , LO-phonon energy $\hbar\omega_{\text{LO}}$, phonon number n , and polaron damping rate Γ , in the bulk at 300 and 120 K. For AlAs, we assume the effective mass of GaAs.

| | α | $\hbar\omega_{\text{LO}}$ (meV) | 300 K | | 120 K | |
|------|----------|------------------------------------|-------|----------------|-------|----------------|
| | | | n | Γ (meV) | n | Γ (meV) |
| GaAs | 0.07 | 36.2 | 0.32 | 0.83 | 0.031 | 0.079 |
| AlAs | 0.11 | 50.1 | 0.17 | 0.89 | 0.008 | 0.041 |

where $\mathbf{q}=(q_{\parallel},q_z)$ is the wave vector of bulk phonons, $M(\mathbf{k}_{\parallel},l;\mathbf{k}_{\parallel}\pm\mathbf{q}_{\parallel},l';q_z)$ is an electron-optical-phonon matrix element between initial state $(\mathbf{k}_{\parallel},l)$ and final state $(\mathbf{k}_{\parallel}\pm\mathbf{q}_{\parallel},l')$, and $\theta(\mathbf{k}_{\parallel},\mathbf{k}_{\parallel}\pm\mathbf{q}_{\parallel})$ is the angle between \mathbf{k}_{\parallel} and $\mathbf{k}_{\parallel}\pm\mathbf{q}_{\parallel}$. The relaxation-time approximation is known to give only a crude estimate of the mobility for scattering from polar optical phonons,³⁴ but is expected to be sufficient for the present purpose in which we are interested only in the relative difference between SQW and WFMSQW.

III. NUMERICAL RESULTS

Figure 2 shows the layer-thickness dependence of the mobility at 300 K in SQW and WFMSQW. The electron sheet density, $N_s=\sum_l N_l$, is $2\times 10^{11}\text{ cm}^{-2}$. For WFMSQW, the thickness of each thin barrier layer is kept constant and their spacing is varied in proportion to the thickness d of the quantum well. The mobility of SQW has a sharp peak at $d=136\text{ \AA}$ and becomes nearly independent of the thickness with small oscillations for $d>200\text{ \AA}$. In WFMSQW, there is a sharp peak at $d=102\text{ \AA}$ and a large and broad peak at $d=543\text{ \AA}$.

At 300 K the electron distribution is classical and electrons are thermally distributed in energy roughly up to about $k_B T$, where k_B is Boltzmann's constant. Consequently, the appearance of intersubband scattering due to phonon absorption into the subband l is roughly determined by the condition

$$\hbar\omega_{LO}+k_B T \gtrsim E_{l1} \equiv E_l(0) - E_1(0). \quad (3.1)$$

In Fig. 3 we show the layer-thickness dependence of the electron mobility at 300 K (same as in Fig. 2) and subband energies measured from the bottom of the lowest subband E_{l1} for (a) SQW and (b) WFMSQW. It is clear that the mobility peak roughly corresponds to the thickness where Eq. (3.1) is satisfied.

For the layer thickness smaller than the first peak ($d\sim 102\text{ \AA}$), the mobility in WFMSQW is larger than

that in SQW. This enhancement is the result of the reduction in the electron-phonon interaction due to the wave-function modulation. Unfortunately, however, this enhancement disappears quickly once the strong intersubband scattering starts to play a role, and the mobility of WFMSQW becomes smaller than that of SQW for $d>120\text{ \AA}$.

In SQW, intersubband scattering starts to be important around $d=136\text{ \AA}$ corresponding to the mobility peak. For thicker SQW's, the thickness where the condition (3.1) starts to be satisfied for subband l increases linearly with l . Consequently, there is essentially no special range of layer thickness for which the mobility can be particularly enhanced and the mobility is nearly independent of $d>200\text{ \AA}$. In WFMSQW, the presence of large intersubband scattering due to barrier-layer insertion reduces the mobility below that in SQW for $120<d<350\text{ \AA}$. Because no new intersubband scattering contributes, the mobility increases continuously in the region $250<d<540\text{ \AA}$ and exceeds that of SQW around $d\sim 350\text{ \AA}$.

The peak mobility of WFMSQW at $d=543\text{ \AA}$ is two

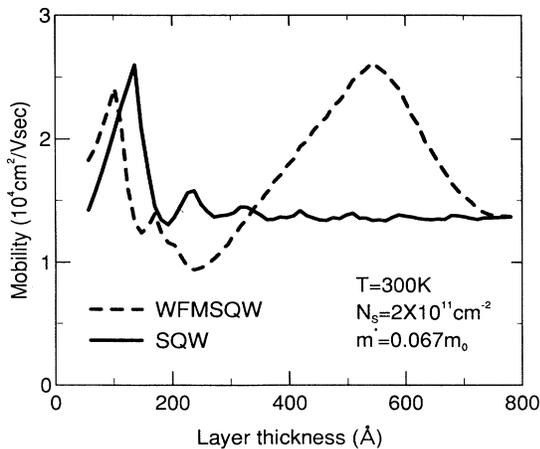


FIG. 2. Calculated mobility as a function of the layer thickness in SQW (solid line) and WFMSQW (dashed line) at 300 K.

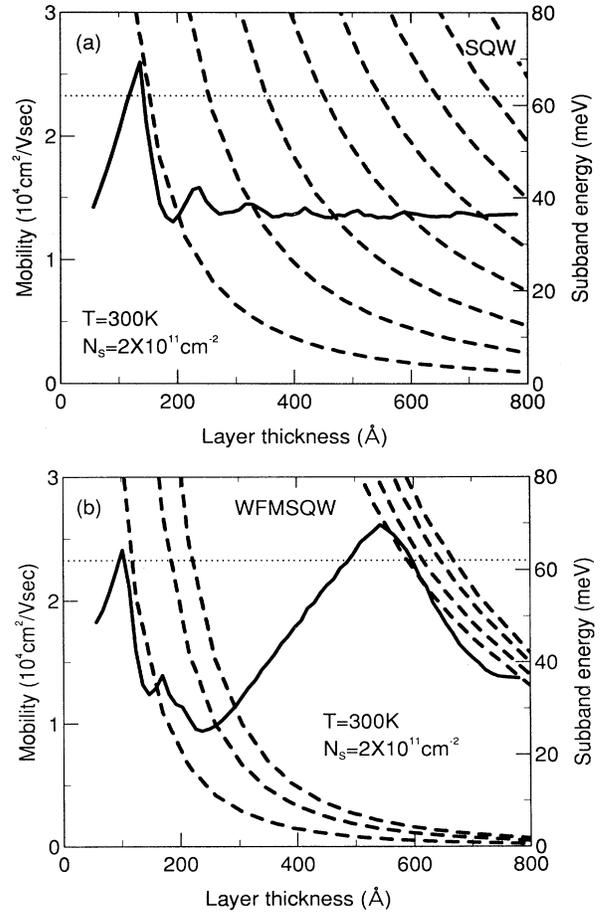


FIG. 3. Calculated subband energy measured from the bottom of the lowest subband (dashed lines) and mobility (solid line) as a function of the layer thickness. (a) SQW and (b) WFMSQW.

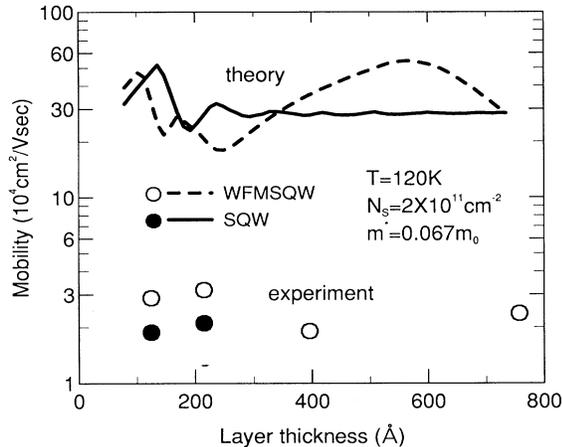


FIG. 4. Calculated and observed mobility at $T=120$ K. The solid and dashed lines show the calculated mobility in SQW and WFMSQW, respectively, and the filled and open circles show the measured mobility in SQW and WFMSQW, respectively.

times as high as that in SQW with the same layer thickness and is nearly the same as that of SQW at 136 Å. This is to be expected because four miniwells become nearly independent of each other for sufficiently thick WFMSQW's. In fact, for $d=543$ Å, the thickness of each miniwell is 127 Å, only slightly smaller than that of SQW corresponding to the mobility peak.

In Fig. 4 the results of the calculation at $T=120$ K are compared with the experiments of Zhu *et al.*³³ The theoretical result is almost one order of magnitude larger than the experimental result. This is partly because of the present relaxation-time approximation which gives rather inaccurate mobility. However, the most significant cause of the discrepancy lies in the fact that the measured mobility is much lower than the known mobility in such systems.³⁵ The measured mobility in WFMSQW is ~ 1.5 times as large as that in SQW for $d=124$ Å, where the calculation gives a lower mobility in WFMSQW than in SQW. The same is applicable to $d=210$ Å.

As the bulk-phonon model is used in the present calculation, the calculated scattering rate may be slightly

overestimated for WFMSQW in which the number of optical phonons in the thin AlAs layers inserted is smaller than that in the GaAs layer. A rough estimate of the scattering rate may be obtained by making an arithmetic average of the Γ 's given in Table I weighted by the relative thickness of the GaAs well layer and the thin AlAs inserted layers. This leads to an enhancement of the mobility only by about 16% at most over the present result for WFMSQW, which does not change the conclusion that the mobility for WFMSQW is smaller than that for SQW at $d=124$ and 210 Å. Zhu *et al.* suggested that the observed enhancement of the mobility in WFMSQW is due to modulation of optical phonons. This is quite unlikely, however. Although individual phonon modes can be strongly modified by the presence of heterointerfaces, their completeness leads to the scattering strength independent of the modification as has been discussed in the previous section. A more detailed calculation is highly desirable to settle this intriguing problem.

IV. SUMMARY AND CONCLUSION

A mobility enhancement through the electron wavefunction modulation was proposed and tested in actual numerical calculations. A wave-function modulation gives rise to two competing effects on the mobility. The first is the reduction in the strength of the electron-phonon interaction, leading to a mobility enhancement, and the second is the introduction of intersubband scattering, leading to a mobility reduction. An appreciable amount of the mobility enhancement can be achieved for appropriate values of parameters for which intersubband scattering is reduced as much as possible.

ACKNOWLEDGMENTS

One of the authors (T.T.) would like to thank Dr. T. Mimura, Dr. M. Abe, Dr. K. Hikosaka, and Dr. K. Joshin of Fujitsu Laboratories Ltd. for continuous encouragement. This work was supported in part by the Industry-University Joint Research Program "Mesoscopic Electronics" and by a Grant-in-Aid for Scientific Research on Priority Area "Electron Wave Interference Effects in Mesoscopic Structures" from the Ministry of Education, Science and Culture, Japan.

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