Direct calculation of the transport properties of disordered AlAs/GaAs superlattices from the electronic and phonon spectra

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We have calculated from first principles the recently measured electron and hole transport of disordered AlAs/GaAs superlattices, in which the individual layer thicknesses $n,m,n8,m8$

this stage, we used computational supercells of up to 1000 ML total length to simulate the AlAs/GaAs *d*-SL. Our main findings were:[6] ~i! all states are localized along the disorder *z* axis, ~ii! the band gap is reduced by about 100 meV ~redshift of PL!, and ~iii! the near-edge optical transition between lo-

$P(i,j)$ denote the probability of an electron hopping from state i to state j, and let $W(i\vec{k},j\vec{k}8)$ be the probability of hopping from substate $(i,\vec{k})$ to another substate $(j,\vec{k}8)$. Then,

$$P\sim i,j!5\sum_{k}\sum_{k8} f_{ik}\sim 1\,2\,f_{jk8}!W\sim i\vec{k},j\vec{k}8!, \qquad \sim 1!$$

where f_{ik} is the occupation of substate $(i,\vec{k})$. For low carrier density, nondegenerate cases, and by assuming equilibrium among the substates $(i,\vec{k})$ within each state i ~reached within picoseconds due to the existence of $\vec{k}$-continuous energy levels!, we have

$$f_{ik}5\frac{2p b\backslash^2}{S_{xy}m}e^{2\sim\backslash^{2/2m}!k^2 b}, \qquad \sim 2!$$

where $b5 1/k_BT$ and T is the temperature and S_{xy} is the x,y cross-section area of the SL. Because f_{ik} is much smaller than one ~nondegenerate case!, we can change Eq. ~1! to

$$P\sim i,j!5\sum_{k}\sum_{k8} f_{ik}W\sim i\vec{k},j\vec{k}8!. \qquad \sim 3!$$

$W(i\vec{k},j\vec{k}8)$ can be calculated by the Fermi golden rule:

$$W\sim i\vec{k},j\vec{k}8!5\frac{2p}{\backslash}\sum_{\mathbf{q}} \mathbb{u}C\sim q!\mathbb{u}^2\wedge i\vec{k}\mathbb{u}\exp\, i\sim\mathbf{q}\ \mathbf{r}!\ \mathbb{u}j\vec{k}8\&^2$$

$$3\,\$N_q o@E\sim i,\vec{k}!\,2\,E\sim j,\vec{k}8!\,1\,\backslash\, v_q\#$$

$$1\sim 1\,1$$

ever, be added back trivially if needed!. Figures 3 and 4 suggest the following observations.

~i! Comparison of the distances traveled by electrons and holes ~at T . 77 K and t . $10^{2\,10}$ sec! in Fig. 4~a! and Fig. 4~b!, respectively, shows that the hole is more mobile than the electron. This reflects the larger hole density of states in the system.

~ii! Inspection of the low T curves shows that there is a characteristic baseline T ! 0 curve both for the $E(t)$ and $\bar{d}^2(t)$ functions. These curves reflect the result of downhill hopping ~i.e., i hops to j when E_i . E_j even if T ! 0). At short times, the curves for all temperatures follow this baseline curve.

~iii! For finite temperature T, the $E(t)$ and $\bar{d}^2(t)$ curves deviate from their baseline curves only after a critical time t_c. This indicates that uphill hopping with phonon absorption takes place for t . t_c.

~iv! For T5 300,150 K ~for electrons! and T5 300,150,77 K ~for holes!

arrows in Figs. 3 and 4!, the electron and hole lose energy very quickly ~Fig. 3!. This is the time scale characteristic of optical phonons. After the first few picoseconds, the energy drops much slower. At the end of these few picoseconds, the electron ~hole! has moved an averaged distance of 77 ~42! ML. This distance is larger for electrons than holes, because the electron has a smaller density of state, thus it has to find more distant states to hop to. Note that 77 ~42! ML are comparable to the effective localization length of the electronic states ~Fig. 1!. After this initial stage, the electron and hole are trapped in local energy minima and thus move much slower.

~viii! In the typical range of time resolved PL experiments[5] ~nano to microseconds

$t(E_{\rm cut}) = t$ determines a cutoff energy $E_{\rm cut}$ in the electron energy distribution, above which there is no electron occupation. The total diffusion constant $D(t)$ is dominated by a small fraction of the electrons at the highest energy. Thus, $D(t) \sim D(E_{\rm cut})$. But $t = t(E_{\rm cut}) \propto 1/D(E_{\rm cut})$, so $D(t) \propto 1/t$. This argument can be applied only to low temperatures when all the hopping events are purely downhill.

B. The $1/t^{1-b}$ regime and the possibility of continuous-time random walks

When $D(t)$ deviates from the $1/t$ curve, it can be described by $1/t^{1-b}$. Such scaling is often discussed in terms of continuous-time random walks ~CTRW!.[31] In the CTRW model, a hopping probability distribution function $c(t_1) \sim t_1^{-(1+b)}$ is assumed and a time-of-flight experimental current $I(t) \propto t^{-(1-b)}$ is obtained. Physically, $I(t)$ is proportional to $D(t)$ through a constant factor. It would thus appear that the CTRW can be used to describe our results. There are a few reasons to think otherwise.

~i! In the CTRW model, $c(t_1)$ describes the probability distribution of the *next* hopping after a given hopping event (t_1 is measured from the absolute time t of the current hopping event!. The average hopping distance is a constant d, independent of how many times the electron has hopped and when ~i.e, at what t_1 in $c(t_1$

T/T_0, which is a CTRW result of a multiple trapping model with an exponential density of state tail $\exp(2E/k_BT_0)$ below a physical mobility edge.[31]

Finally, ~iii! in the CTRW $c(t_1) ; t^{2(1-b)}$ model, the system reaches equilibrium only at $t \to \infty$ for exponentially decaying, unbound DOS, thus $D(t)$ will follow the $1/t^{1-b}$ scaling forever ~in the exponential density of state tail model, for $T < T_0$, the equilibrium state corresponds to an energy distribution infinitely deep which will take an infinitely long time to reach!. In reality, of course, given long enough time the system will reach equilibrium @see Sec. V items ~iv! and ~v!#. Thus, the $D(t) \sim 1/t^{1-b}$ scaling will give way to a constant ~horizontal line!. This happens in our simulation at $T = 300,150$ K for electrons and at $T = 300,150,77$ K for holes. Based on the above arguments, we conclude that one cannot use the $D(t) \sim 1/t^{1-b}$ scaling to justify the validity of the CTRW.

$$I(t) = I_0 \exp\left[-\alpha \int_0^t \left(D_{el}(t) + D_{hole}(t)\right) dt / t_a\right]$$

$$= I_0 \exp\left[-\frac{\alpha}{2}\left(\bar{d}^2_{el}(t) + \bar{d}^2_{hole}(t)\right) / t_a\right]. \qquad (11)$$

Note that in the exponential, only one term dominates at a given time range. At the experimental time range of nanoseconds to microseconds, for T less than 300 K, the $D_{el}(t)$ and $D_{hole}(t)$ are described by $1/t^{1-b}$, thus $\bar{d}^2_{el}(t)$ and

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APPENDIX A: THE FORMULAS FOR $P_{i,j}$

For the *optical-phonon polar* effect:

$$P_{\mathrm{OPP}}(i,j) = f_{\mathrm{OPP}}$$

find that if E_i . E_j by an amount larger than $\backslash v_0$, then $P_{\mathrm{OPP}}(i\ !\ j)$ has the largest contribution of all P's at all temperatures. If E_i is not larger than E_j by $\backslash v_0$, then ~i! at high temperature (T . 100 K!, P_{OPP} has the largest contribution, ~ii! at lower temperature (T , 100 K! and for small $E_j 2 E_i$ if E_j . E_i, P_{APP} has the largest contribution, followed by P_{APD} ~a factor of 2–10 smaller than P_{APP}).

The parameters used in Eqs. ~A1!,~A8!, and ~A10! are the following. Some of them are from calculations[13] and others from experimental results.[39] $P 5 (2 0.32 2 0.45)/2$ C/m^2, $\backslash v_0 5 (36 1 50)/2$ meV, e_0(GaAs) 5 12.85, e_0(AlAs) 5 10.06, e_∞(GaAs) 5 10.89, e_∞(AlAs) 5 8.16, C_1(el) 5 (11.38 1 10.56)/2 eV, C_1(hole) 5 (2.7 1 2.6)/2 eV, m(el) 5 (0.077 1 0.158)/2 electron mass, m(hole) 5 (0.416 1 0.439 1 0.079 1 0.157)/4 electron mass, $C_s^L 5 (36 1 44)/2$ meV/$q_{\max}$, $C_s^T 5 0.58 C_s^L$, $q_{\max} 5 2p/10.6826$ bohrs^{21}. In the averages, the first number is the value of GaAs, the second number is for AlAs.

[1] A. Chomette, B. Deveaud, A. Regreny, and G. Bastard, Phys. Rev. Lett. **57**, 1464 ~1986!.

[2] A. Sasaki, M. Kasu, T. Yamamoto, and S. Noda, Jpn. J. Appl. Phys. **28**, L1249 ~1989!.

[3] L. Pavesi, E. Tuncel, B. Zimmermann, and F. K. Reinhart, Phys. Rev. B **39**, 7788 ~1989!.

[4] M. Kasu, T. Yamamoto, S. Noda, and A. Sasaki, Jpn. J. Appl. Phys. **29**, L1588 ~1990!.

[5] D. J. Arent, R. G. Alonso, G. S. Horner, D. Levi, M. Bode, A. Mascarenhas, J. M. Olson, X. Yin, M. C. DeLong, A. J. Spring Thorpe, A. Majeed, D. J. Mowbray, and M. S. Skolnick, Phys. Rev. B **49**, 11 173 ~1994!.

[6] K. A. Mäder, L.-W. Wang, and A. Zunger, Phys. Rev. Lett. **74**, 2555 ~1995!.

[7] K. A. Mäder, L.-W. Wang, and A. Zunger, J. Appl. Phys. **78**, 6639 ~1995!.

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