Applied Bias Slewing in Transient Wigner Function Simulation of Resonant Tunneling Diodes

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***Abstract*—The Wigner function formulation of quantum mechanics has shown much promise as a basis for accurately modeling quantum electronic devices, especially under transient conditions. In this work, we demonstrate the importance of using a finite applied bias slew rate (as opposed to instantaneous switching) to better approximate experimental device conditions, and thus to produce more accurate transient Wigner function simulation results. We show that the use of instantaneous (and thus unphysical) switching can significantly impact simulation results and lead to incorrect conclusions about device operation. We also find that slewed switching can reduce the high computational demands of transient simulations. The resonant tunneling diode (RTD) is used as a test device, and simulation results are produced with SQUADS (Stanford QUAntum Device Simulator).**

I. Introduction

THE WIGNER function formulation of quantum mechanics has proven to be a very effective basis for the numerical simulation of quantum electronic devices under transient conditions in self-consistent, dissipative, and open-boundary systems [1]–[7]. However, the necessary iterative solution of the Wigner function transport equation is very compute intensive, resulting in the classic trade-off between the accuracy and efficiency of the numerical implementation. We have identified a technique for transient Wigner function simulation that achieves the unlikely combination of improving both accuracy and efficiency—using a finite applied bias slew-rate (the rate at which the applied bias is changed with respect to time). To our knowledge, all transient Wigner function simulations of quantum devices to date have used instantaneous changes in the applied bias. Step function inputs result in simpler simulator code and fewer simulation parameters to choose or investigate. However, we show in Section II that the use of an infinite (and thus unphysical) slew rate can significantly impact simulation results and lead to incorrect conclusions about quantum device operation.

Before discussing slew rates directly, we consider the physics of transient bias switching in some detail [8]. In a transient simulation, applied bias changes are completed during a time step (i.e., between consecutive solutions of the system). Changing the applied bias across a device requires a current pulse in the external circuit, essentially "communicating" the new bias to the device. If the applied bias is changed too quickly for free carriers in the device to respond to this current pulse, the bias change is effectively instantaneous, and the external current simply charges the contacts, producing an electrostatic field across the device. In other words, the device acts like a capacitor. For a one-dimensional "capacitor" of area A, width L, and permittivity ε, the external current density $J_{\rm ext}$ necessary to cause a voltage change ΔV in time Δt is

$$J_{\rm ext} = \frac{I_{\rm ext}}{A} = \frac{\Delta Q}{A\Delta t} = \frac{C\Delta V}{A\Delta t} = \frac{\varepsilon\Delta V}{L\Delta t}. \tag{1}$$

$J_{\rm ext}$ occurs entirely within the time step Δt. Following a bias change, free carriers will respond over time to the electric field as they redistribute, enter, and leave the device to accommodate the new applied bias.

To maintain physical correctness, our quantum device simulator, SQUADS [7], implements the above described behavior in self-consistent, transient simulations. That is, because time steps are typically on the order of 1 fs, applied bias changes of any magnitude during a time step are effectively instantaneous, and therefore initially appear as electrostatic fields across the entire device. SQUADS computes and prints the average external current $J_{\rm ext}$ required to produce the specified bias change in a single time step, although this current does not appear in any of the simulated internal device currents. Enforcing self-consistency through the Poisson equation naturally causes free carriers in the device to respond appropriately over time to the electric field. Note that slewing the applied bias is accomplished simply by making many small, "instantaneous" bias changes during consecutive small time steps. [In this manuscript, "instantaneous" means "single time step".] Given the above description of how transient bias changes should be implemented in a device simulator, we can now demonstrate the significance of the applied bias slew rate in transient Wigner function simulations.

II. Results and Discussion

A. Simulated Device and Operation Summary

Resonant tunneling diodes (RTD's) have served as an excellent quantum device simulation test-bed, since they have a relatively simple structure and biasing configuration, their quantum effects are strong, and experimental results (for comparison to simulation) are plentiful. The particular RTD used in this work (see Fig. 1) was selected because of the strong transient effects it displays, as discussed by Jensen and Buot [9] and in our previous work [7]. Fig. 2 shows the steady-

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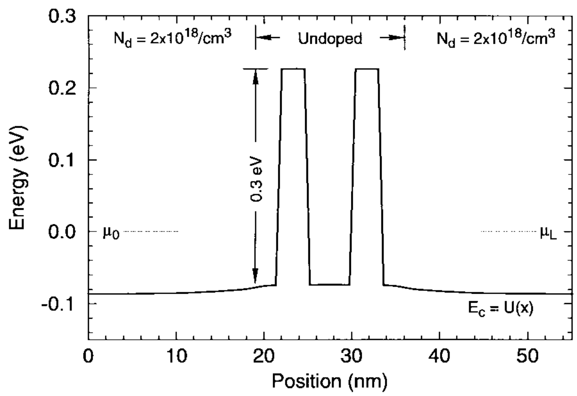

Fig. 1. Simulated GaAs RTD structure: equilibrium self-consistent conduction band, Fermi levels, and doping. The 0.3 eV $Al_{0.3}Ga_{0.7}As$ tunnel barriers are 3 nm thick, and the GaAs quantum well width is 5 nm. The center 17 nm of the device (including 3 nm outside each tunnel barrier) are undoped.

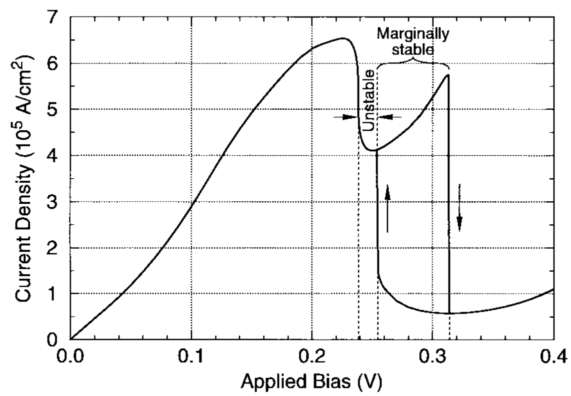

Fig. 2. Self-consistent, steady-state RTD $I-V$ curve showing negative differential resistance, hysteresis, and bistability. The RTD is unstable (oscillates perpetually) in the plateau between 0.239 V and 0.254 V, and it is marginally stable (oscillates with slow damping) in the remainder of the plateau.

state self-consistent $I-V$ curve for this RTD as simulated by SQUADS. Previous transient simulations [7] showed that this RTD is stable at all points on this $I-V$ curve except in the plateau (0.239 V–0.313 V on the up-trace and 0.254 V–0.239 V on the down-trace). Where the two traces coincide in the plateau (0.239 V–0.254 V), perpetual high-frequency ($\sim$2.5 THz) current oscillations occur. In the remainder of the plateau on the up-trace, the RTD is only marginally stable (it approaches steady-state in a weakly-damped oscillatory fashion). Since the most interesting transient phenomena occur in the plateau region of the $I-V$ curve, transient simulations of this region offer a very effective means of analyzing the effects and importance of slew rate variation.

All transient simulations in this work used the Cayley transient operator [10], [7] with a 1 fs time step. The Gummel iteration method was used to implement self-consistency [7]. For $I-V$ curve simulations, operating points were taken every 10 mV. Three convergence criteria were used to determine when steady-state had effectively been reached after applied bias changes: potential change less than 10^{-6} eV, Poisson equation satisfied to less than 10^{-8} eV, and current variation across the device of less than 1000 A/cm^2.

B. Instantaneous Bias Switching

To determine the effects of slew rate on simulation results, we first ran a transient $I-V$ curve simulation using the standard approach of instantaneous bias switching. Thus, starting from a steady-state solution at one bias, the applied bias was changed to the next bias point in a single time step, and the system was again allowed to evolve to steady-state. After each bias switch, a very large current pulse of about 1.5×10^5 A/cm^2 peak amplitude and about 50 fs duration occurred. The amplitude of this current pulse often exceeded both the starting and ending currents. For example, Fig. 3 shows the transient position-averaged current and the collector contact current in the RTD after instantaneous switching from 0 V to 10 mV. [Hereafter, all currents will be position-averaged values, since this is the current induced in the external circuit.] Note that the peak current is seven to eight times the final steady-state value. During the down-trace, the current pulse was negative, but with essentially the same amplitude and duration. Based on the consistency of the current pulse in amplitude and duration throughout the $I-V$ curve trace (except at bistable points), simple computations [11] confirmed that the pulse resulted from charging of the accumulation and depletion layers to accommodate the 10 mV change in applied bias between bias points.

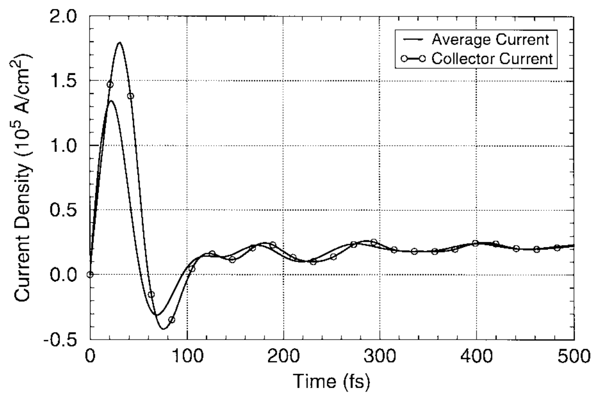

Fig. 3. Transient position-averaged current (plain curve) and collector contact current (circle curve) after switching from 0.0 V to 10 mV. Note that the peak of the current pulse is seven to eight times the final value.

The origin of the current pulse described above has been the source of some consternation in the past. For example, Tsuchiya *et al.* [12] attempted to explain the current pulse in a transient Wigner function simulation after a bias switch across the negative differential resistance (NDR) region of the $I-V$ curve in terms of the discharging of the quantum well and the properties of the electrodes (emitter and collector layers). Similarly, Kluksdahl *et al.* [4] suggested that "the overshoot probably arises from a rapid discharge of the trapped charge in the potential well." Simple calculations [11] show that the quantum well charge in these cases was much too small to produce the observed current pulse, while the required change in accumulation and depletion charge was about right. Use of a finite slew rate in these instances (or switching the bias outside the NDR region) would have shown that the current pulse was largely due to the charging of the accumulation and depletion layers. Thus, instantaneous bias switching in transient Wigner function simulations may obscure device operation to the extent that incorrect conclusions are drawn. [Note that in the earlier work of Frensley [1], nonself-consistent, transient Wigner function simulations also showed a current pulse after switching an RTD across the NDR region. However, in this case Frensley's conclusion that the pulse was due to the charging or discharging of the quantum well was correct. Since Frensley did not enforce self-consistency, there would be no accumulation and depletion charges.]

Much worse than the internal current pulse from a practical standpoint is the external circuit current $J_{\rm ext}$ required to change the bias by 10 mV in a single time step (although $J_{\rm ext}$ does not appear in any simulation results). Using (1), with $L = 55$ nm, $\varepsilon = 12.9\varepsilon_o, \Delta V = 10$ mV, and $\Delta t = 1$ fs, the external current density is $J_{\rm ext} = 2.1 \times 10^6$ A/cm^2 for this RTD. This is at least three times larger than any current the external circuit must supply for steady-state device operation anywhere in the simulated bias range (see Fig. 2). In summary, the use of instantaneous bias switching in self-consistent quantum device simulation produces a huge current pulse within the device, and it would require an even larger current spike from the driving source. Neither of these represent practical quantum system behavior in real measurement or circuit environments.

C. Realistic Slew Rates

The above simulations show that instantaneous bias switching in transient Wigner function simulations presents a huge "shock" to the quantum device, resulting in a large internal current pulse and damped oscillations thereafter, as shown in Fig. 3. To more accurately model the operation of real quantum devices and circuits, a finite applied bias slew rate must be used. Based on the simulation results above, RTD-type devices can respond and change state in about 100 fs, so 100 fs bias slewing seems appropriate for studying how an RTD might operate in a circuit of its peers. A second transient $I-V$ curve simulation was therefore conducted at a slew rate of 10 mV/100 fs (100 V/ns). As an example, Fig. 4 shows the transient current for the slewed switch from 0 V to 10 mV, along with the same plot for instantaneous switching. Note that the accumulation/depletion charging current pulse (which must have the same integral over time, or total charge transfer) of $J_{DA} \approx 4 \times 10^4$ A/cm^2 is much less severe with slewed switching. Also, (1) gives an external current of only $J_{\rm ext} = 2.1 \times 10^4$ A/cm^2. Neither of these are large compared to normal operating currents of the device, which confirms that this slew rate could reasonably occur in a quantum circuit.

The use of 100 V/ns slewed switching in transient Wigner function simulations, while improving the accuracy of the simulation, had the ancillary benefit of reducing their very high computational cost. The shock of instantaneous bias switching required a relatively long transient simulation before the convergence criteria were satisfied (i.e., steady-state was reached). Slewed switching lessened the shock, so that, although reaching the next bias took longer, total time to steady-state was much less. For example, for the 0 V to 10 mV switching simulation shown in Fig. 4, steady-state was reached in 330 fs with slewing, versus 550 fs without. On average, convergence

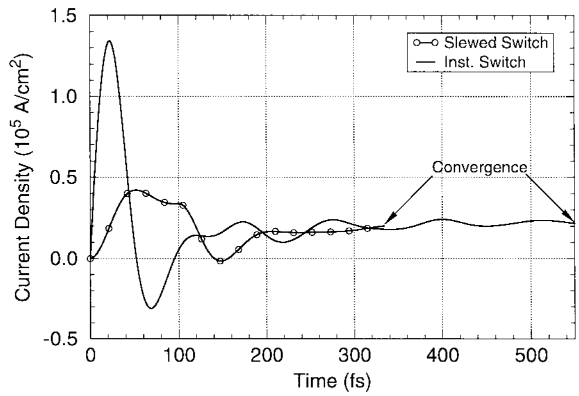

Fig. 4. Transient current after switching from 0.0 V to 10 mV. The plain curve shows the transient current when the bias is switched instantaneously; the circle-curve shows the same when the bias is slewed from 0.0 V up to 10 mV over 100 fs. Note that the slewed switching simulation reaches steady-state significantly faster than the instantaneous switching simulation.

was reached about 20% faster with slewed switching, even in the critical plateau region (where thousands, rather than hundreds, of femtoseconds were required for convergence). Needless to say, a 20% improvement in computation time is very significant in a several-hundred hour simulation task. [Note that if transient effects are not specifically of interest, much more computationally efficient steady-state simulation methods [7] can be used.]

The 100 V/ns slew rate was chosen to model an RTD driven by an equally fast device. If simulation results are to be compared to RTD measurements by a device tester, an even lower slew rate is appropriate. Fast operational amplifiers (which might serve as the front end for a device tester) are capable of perhaps 2000 V/μs slew rates [13]. Taking 1 V/ns as potentially feasible value, this is a factor of 100 lower than the slew rate used above, and would require 10 ps (10 000 time steps) to change the applied bias by 10 mV. The question is, if one wished to simulate experimental device test conditions (e.g., to test simulator accuracy), is it necessary to go to such a huge expense? In other words, given the instantaneous switching and 100 V/ns slewing simulation results, can lower slew rate effects be estimated by extrapolation or even neglected (i.e., steady-state operation assumed)? In this case, the answer is no. Simulation results in the following section indicate that when the details of *this* device's operation are being investigated, there are cases where even a 1 V/ns slew rate is too high.

D. Intrinsic Oscillations

As stated earlier, the most interesting transient effects for the chosen RTD occurred in the plateau region of its $I-V$ curve. We therefore investigated in more detail the effects of slew rate variation in this region of operation. In tracing the $I-V$ curve in the plateau, both instantaneous and 100 V/ns slewed switching initiated oscillations that persisted for thousands of femtoseconds (at 1 fs per time step). These oscillations were so persistent that Jensen and Buot [9] concluded that the RTD oscillated perpetually at all biases in the plateau, and that these oscillations were necessary for the plateau's existence. However, we showed in previous work [7] that

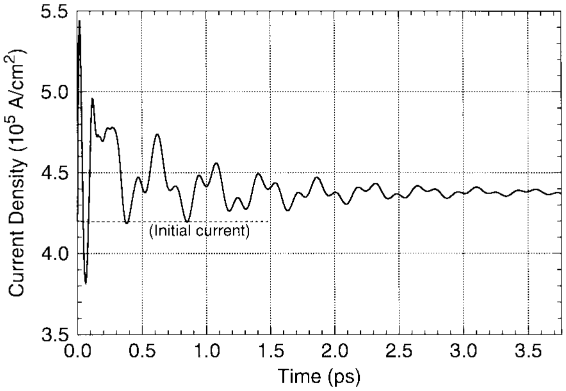

Fig. 5. Transient current after instantaneous switching from 0.26 V to 0.27 V in the plateau. Although the difference between initial and final current is less than 2×10^4 A/cm^2, the oscillation amplitude starts at ten times this value. The oscillations are initiated by the abrupt switching.

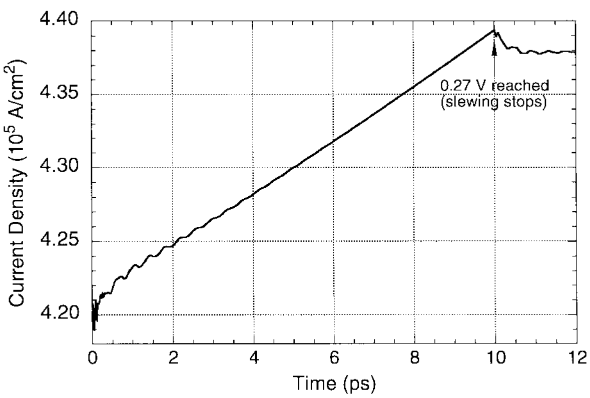

Fig. 6. Transient current during and after 10 ps slewing from 0.26 V to 0.27 V in the plateau (slew rate: 1 V/ns). Although small oscillations occur even at this low slew rate, the oscillation amplitude is less than 1/100th of that in Fig. 5.

this RTD is only truly unstable in the plateau between 0.24 V and 0.25 V. [Further simulations [14] marked the unstable region more precisely at between 0.239 V and 0.254 V.] Above this range in the plateau, the oscillations eventually decayed to steady-state. For example, Fig. 5 shows the current after instantaneous switching from 0.26 V to 0.27 V. Since the RTD is stable (albeit marginally so) at applied biases above 0.254 V, these oscillations were apparently initiated by the abrupt bias changes. A 1 V/ns slew rate (10 000 time steps per 10 mV) simulation from 0.26 V to 0.27 V was conducted to verify this. The result is shown in Fig. 6. Even this simulation shows very small oscillations after the (abrupt) start and end of slewing. Presumably, even lower slew rates would avoid oscillations entirely. Thus, once again the use of an infinite slew rate (by Jensen and Buot) has been a culprit in producing simulation results which led to invalid conclusions about device operation.

A further set of simulations sought to determine the effect of slewing the applied bias smoothly through the unstable region of operation. This might occur in the simulation of a device with an unstable region that was smaller than the chosen bias step. In this case, the existence of oscillations would probably be missed entirely. Transient simulations starting at 0.23 V and slewing the bias continuously to 0.26 V served to investigate this possibility. The results are shown in Fig. 7.

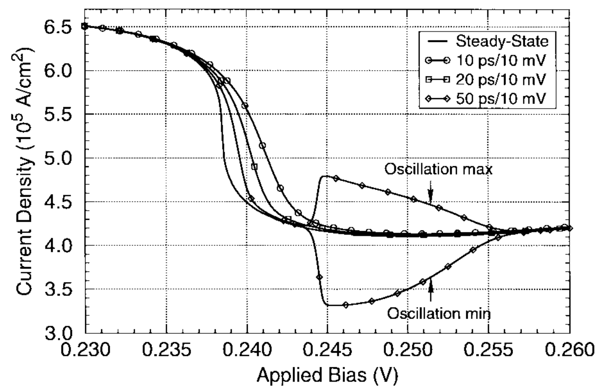

Fig. 7. Trace of unstable region of $I-V$ curve. Continual slewing at 1 V/ns (or 10 ps/10 mV) and 0.5 V/ns (or 20 ps/10 mV) are too fast to allow the RTD to begin oscillating before it leaves the unstable region at 0.254 V. Continual slewing at 0.2 V/ns (or 50 ps/10 mV) is slow enough. Only the peaks of the oscillation are shown, so that the other curves are not obscured.

At 1 V/ns (10 000 time steps per 10 mV), the device slewed through the unstable region too quickly for oscillations to begin. The results was the same at 0.5 V/ns, (20 000 time steps per 10 mV). Finally, at 0.2 V/ns (50 000 time steps per 10 mV), the RTD was able to achieve the conditions necessary for oscillations (described in [14]). The oscillations persisted during the continuous slewing, albeit with decreasing amplitude, until shortly after the unstable region was exited. These results indicate a relatively very slow response time for a device which is otherwise so fast. The lesson is that even the use of a relatively low slew rate may still allow some device physics to be missed.

Since simulation results in the plateau region of the $I-V$ curve depend strongly on the slew rate used, it is again important to consider what might happen in an actual circuit or test environment. Device analyzers (such as the HP 4145) trace an $I-V$ curve by sweeping the applied bias in a step-wise fashion, so that a new bias is established, a delay time (typically a few milliseconds) elapses to allow the device to settle to steady-state, and the current is measured. Thus, with an ideal device tester, oscillations would definitely be seen in the unstable region (assuming at least one bias point fell there), since there would be plenty of time for the device to evolve to the unstable conditions. In the marginally stable region, since the slew rate would be less than 1 V/ns and slewing would start and stop more smoothly, no oscillations would occur after 0.254 V. However, device testers are not ideal. External inductance and capacitance in the measuring apparatus could easily change a marginally-stable RTD into an unstable one, causing the RTD to oscillate everywhere in the plateau. Based on the 100 V/ns simulation results, this RTD would certainly oscillate throughout the plateau in a fast-changing RTD circuit.

E. Bistable Regions

Bistable regions pose yet another hazard for instantaneous bias switching. When a transient simulation is used to trace the steady-state $I-V$ curve (e.g., to search for latent transient effects), for this RTD, instantaneous switching produced the same $I-V$ curve as the steady-state simulation and the slewed-switching, transient simulation. However, it was not difficult

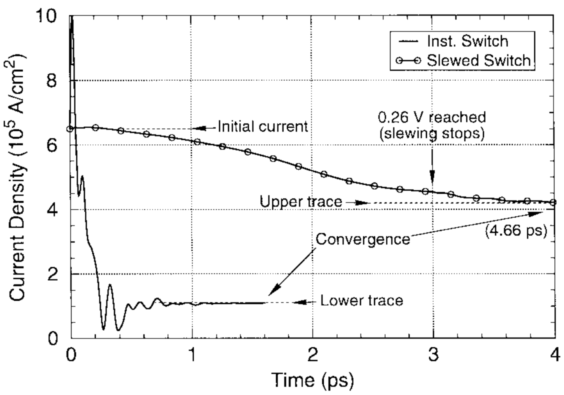

Fig. 8. Transient current after switching from 0.23 V to 0.26 V. The instantaneously switched simulation (plain curve) converged to the lower bistable value, while the 10 V/ns slewed simulation (circle-curve) converged to the upper value. This shows that slew rate variation can profoundly affect device function.

to devise a transient simulation that did not follow the steady-state $I-V$ curve. For example, a transient simulation starting from steady-state at 0.23 V and switching instantaneously into the bistable region at 0.26 V, rather than converging to the "correct" higher current state, converged to the lower current state. In contrast, the same simulation with a 10 V/ns slew rate converged to the higher current state. These results are shown in Fig. 8. Our standard slew rate of 100 V/ns was also too fast to converge to the upper $I-V$ curve trace. In general, the shock of instantaneous, or even fast, bias switching may cause a device to "leap the rails" onto another trace in a bistable or multi-stable region of operation. It should be noted that switching to the "wrong" state might be a useful function (e.g., to achieve a higher effective NDR value or produce a multi-state device). By varying the slew rate in simulations, it is possible to investigate how fast the device must be switched in order to produce this type of device operation.

III. Conclusions

In this work, we have demonstrated the importance of using a finite applied bias slew rate (as opposed to instantaneous switching) to better approximate experimental device conditions, and thus produce more accurate transient Wigner function simulation results. In fact, the proper slew rate for simulations depends on the intended application conditions and the desired device function. We showed several instances where the use of instantaneous switching has led to incorrect conclusions about device operation. As a added benefit, we showed that the use of slewed switching can also reduce the high computational demands of transient simulation.

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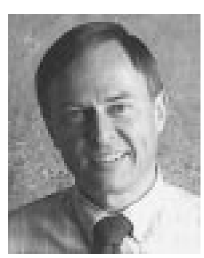

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