Velocity overshoot onset in nitride semiconductors

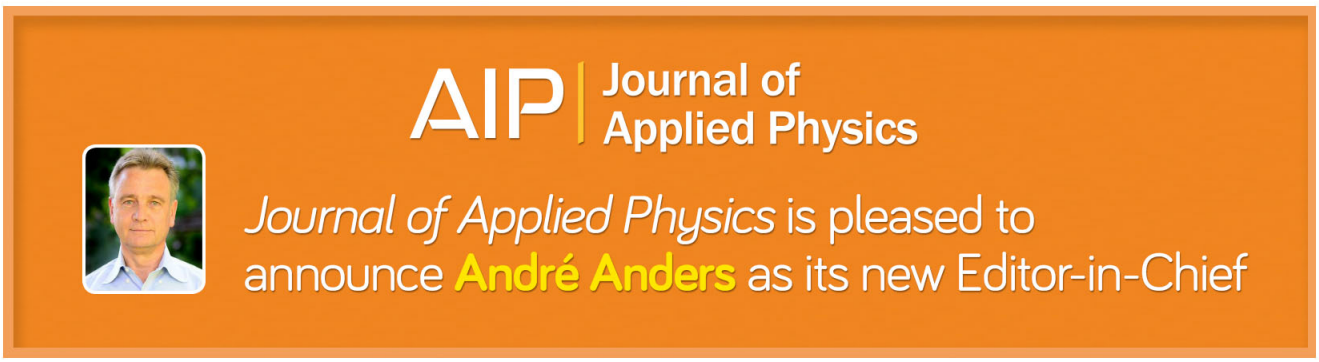
C. G. Rodrigues, V. N. Freire, A. R. Vasconcellos, and R. Luzzi

Citation: Applied Physics Letters **76**, 1893 (2000); doi: 10.1063/1.126203

View online: http://dx.doi.org/10.1063/1.126203

View Table of Contents: http://scitation.aip.org/content/aip/journal/apl/76/14?ver=pdfcov

Published by the AIP Publishing



Velocity overshoot onset in nitride semiconductors

C. G. Rodrigues
Departamento de Matemática e Física, Universidade Católica de Goiás, Caixa Postal 86, Goiânia, Goiás, Brazil

V. N. Freire[a)]
Departamento de Física, Universidade Federal do Ceará, Caixa Postal 6030, Campus do Pici, 60455-760 Fortaleza, Ceará, Brazil

A. R. Vasconcellos and R. Luzzi
Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas, Caixa Postal 6165, 13083-970 Campinas, São Paulo, Brazil

(Received 4 October 1999; accepted for publication 5 February 2000)

A theoretical study on the electron drift velocity and some nonequilibrium thermodynamic characteristics of wurtzite GaN, AlN, and InN is presented. It is based on a nonlinear quantum kinetic theory which provides a description of the dissipative phenomena developing in the system. The ultrafast time evolution of the electron drift velocity and quasitemperature is obtained, and overshoot effects are evidenced on both. The overshoot onsets are shown to occur at 20 kV/cm in GaN, 60 kV/cm in AlN, and 10 kV/cm in InN, electric field intensities which are considerably smaller than those that have been recently derived resorting to Monte Carlo simulations. © *2000 American Institute of Physics.* [S0003-6951(00)03914-0]

Nitride semiconductors like GaN, AlN, and InN have been object of intense research in recent years, a consequence of the large technological interest associated with their applications in blue/UV light emitting diodes and diode lasers (e.g., Ref. 1). Promising characteristics for power field effect devices, high-performance and high-frequency transistors,[2] and the lack of information concerning some of the bulk III-nitrides basic properties have led to the realization of several recent studies on their high-field steady-state transport properties.[3–13] However, only a few of them were concerned with the transient transport regime,[14–16] whose understanding is important for the improvement of nitride-based devices with submicron channels and high cutoff frequency.

The bulk nitride transport properties have been calculated using Monte Carlo simulations and Boltzmann transport equations. In steady-state conditions, negative differential resistivity (NDR) was shown to exist in AlN, GaN, and InN for electric fields with intensities larger than approximately 450, 140, and 65 kV/cm, respectively,[3–13] having a doping concentration of $1.0\times 10^{17}\,\mathrm{cm}^{-3}$ and in contact with a bath at a temperature of 300 K. Those results should be recognized as approximations since they are highly dependent on the details of the band structure parameters as, for example, the effective mass values in the secondary valleys, which are as yet unknown. The transient transport regime in the III nitrides follows in a subpicosecond scale ($<0.3\,\mathrm{ps}$), during which an overshoot in the electron velocity can be evidenced for high enough electric fields. The onset for the electron velocity overshoot in wurtzite GaN was shown by Foutz *et al.*[16] to occur for electric fields higher than 140 kV/cm, while Caetano *et al.*[15] obtained that the electric field should be higher than 50 kV/cm. To date, Foutz *et al.*[16] have been the only ones to calculate the electric field for the onset of the electron overshoot in AlN and InN, obtaining 450 and 65 kV/cm, respectively. These are also the electric field intensities for the existence of NDR in each nitride when the electron effective masses in the secondary valleys are assumed to be the free space electron mass m_0.[16]

Seaking a better understanding of the electron velocity overshoot effect in wurtzite GaN, AlN, and InN, we perform a theoretical study of their transient transport properties resorting to a powerful, concise, and soundly based kinetic theory for far-from equilibrium systems.[17] It is the one founded on a nonequilibrium statistical ensemble formalism, the so-called MaxEnt-NESOM for short,[18] which provides an elegant, practical, and physically clear picture for describing irreversible processes,[19] as for example in semiconductors far-from from equilibrium,[20] which is the case considered here. Through the numerical solution of associate quantum transport equations based on the MaxEnt-NESOM, we characterized the onset of the electron velocity overshoot in wurtzite GaN, AlN, and InN.

To investigate the transport transient behavior in AlN, GaN, and InN, we derive in the MaxEnt-NESOM-based nonlinear quantum kinetic theory the evolution equations for the energy of carriers and longitudinal and acoustic phonons, $E_C(t)$, $E_{LO}(t)$, $E_{ac}(t)$, and the carriers' momentum $\mathbf{P}(t)$ (along similar lines as already applied to the study of transport phenomena in GaAs[21]). Associated with the above quantities are five intensive nonequilibrium thermodynamic variables (the Lagrange multipliers that the variational MaxEnt-NESOM introduces), which are interpreted as related to: time-evolving nonequilibrium temperatures (referred to as quasitemperatures) for carriers and longitudinal optical (LO) and alternating-current (AC) phonons,[20] which we call $T_c^*(t)$, $T_{LO}^*(t)$, and $T_{ac}^*(t)$; the carriers' drift veloc-

a)Electronic mail: valder@fisica.ufc.br

ity $\mathbf{v}(t)$; and a nonequilibrium chemical potential $\mu^*(t)$ (quasichemical potential).

Using the Makovian approximation in the MaxEnt-NESOM based kinetic theory,[17] we find that

$$\frac{d}{dt}E(t) = -\frac{e\mathbf{F}}{m^*}\cdot\mathbf{P}(t) + J_E^{(2)}, \tag{1}$$

$$\frac{d}{dt}\mathbf{P}(t) = -ne\mathbf{F} + \mathbf{J}_P^{(2)}, \tag{2}$$

$$\frac{d}{dt}E_{LO}(t) = -J_{E_{LO}}^{(2)} - J_{LO,AN}^{(2)}(t), \tag{3}$$

$$\frac{d}{dt}E_{ac}(t) = -J_{E_{ac}}^{(2)} + J_{LO,AN}^{(2)}(t) + J_{ac,dif}^{(2)}(t), \tag{4}$$

where n is the doping concentration. The first term on the right of Eq. (1) stands for the energy rate that the external electric field $\mathbf{F}$ transfers to the carriers, while the second is the one taking account of the transfer of excess energy to the phonons. The first term on the right of Eq. (2) is the drifting force provided by the electric field, and the second the rate of change of carrier momentum as a result of collision with phonons. In Eq. (3) we have at the right, first, the rate of change of the LO phonon energy due to their interaction with the carriers; the last term accounts for the relaxation to the acoustic phonons due to anharmonic interactions. In Eq. (4), similarly to Eq. (3), the first term $J_{E_{ac}}^{(2)}$ is the rate of change of the AC phonon energy due to their interaction with the carriers; the second one is the relaxation due to anharmonic interaction with the LO phonons, and the last one is the contribution of thermal diffusion to the reservoir (this latter type of contribution for the case of carriers and LO phonons is very small and has been neglected). A detailed description of these terms can be found elsewhere.[17,21]

We solve numerically the set of coupled nonlinear integrodifferential Eqs. (1)–(4) to obtain the evolution and steady-state behavior of the basic intensive nonequilibrium thermodynamic variables for wurtzite GaN, AlN, and InN. We have used for these materials the characteristic parameters (effective mass, phonon frequencies, Fröhlich coupling strength, deformation potential strength, etc.) available in the literature.[16] The electric field applied to GaN and AlN (InN) is restricted to be smaller than 120 kV/cm (60 kV/cm) since intervalley scattering is not considered in this work. The doping concentration is taken as $1.0\times10^{17}\,\mathrm{cm}^{-3}$, and the bath temperature 300 K, that are the same used by Foutz *et al.*[16] in their calculations.

The evolution of the electron drift velocity and quasitemperature towards the steady state is depicted in Figs. 1 and 2, respectively. These figures permit to characterize the presence of an overshoot in both the electron drift velocity and quasitemperature. The onset of the overshoot effect occurs at 20 kV/cm in GaN, 60 kV/cm in AlN, and 10 kV/cm in InN. An analysis of the different channels of pumping and relaxation allows us to conclude that the overshoot at sufficiently high fields is a consequence of the interplay of energy and momentum relaxation times. No overshoot occurs when the momentum relaxation time, which is smaller than the energy relaxation time shortly after application of the electric field, becomes predominantly larger than the other. On the other hand, the overshoot follows at intermediate to high fields when the relaxation time for energy is constantly larger than the one for momentum. Moreover, it is verified that the peak in velocity follows in the time interval where the drift-kinetic energy $m^*v^2(t)/2$ increases more rapidly than the thermal energy $k_BT_C^*(t)$, and the peak in quasitemperature follows for a minimum of the quotient of these two energies.[17] On the other hand, the smooth overshoot on the carriers' quasitemperature in GaN, AlN, and InN, which was not reported before, is due to the changes of the LO phonons temperature related to the carriers excess energy dissipation,[17] which was not considered by Caetano *et al.*[15] and Foutz *et al.*[16]

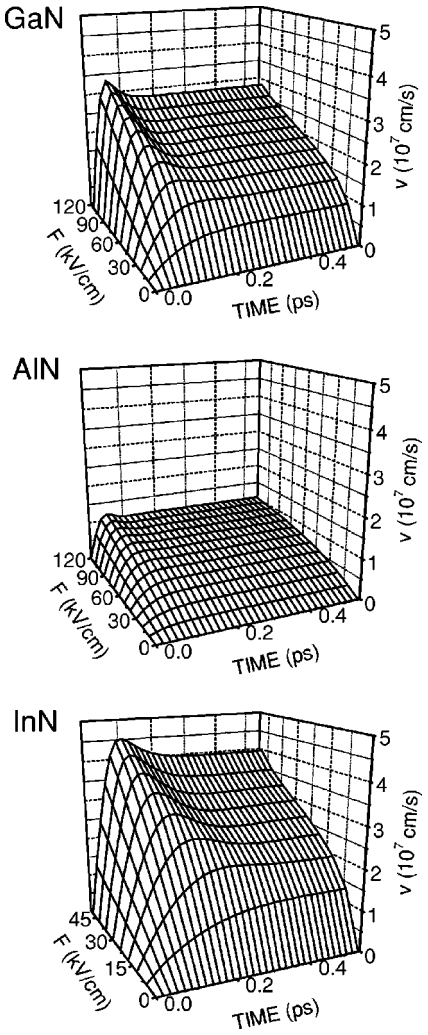


FIG. 1. Time evolution towards the steady state of the electron drift velocity in GaN (upper figure), AlN (middle figure), and InN (lower figure).

The time for the electrons to attain the steady state is in our calculations very approximately the same obtained previously by other authors using different descriptions of the transient transport phenomena.[14–16] The electric field value we have found for the onset of the velocity overshoot in wurtzite GaN agrees very well with that calculated by Caetano *et al.*[15] using energy-momentum balance equations. During the transient regime, however, the mean electron energy (which is directly related to the electron quasitemperature) does not present an overshoot effect in the results of Caetano *et al.*[15] On the other hand, the values of the electric

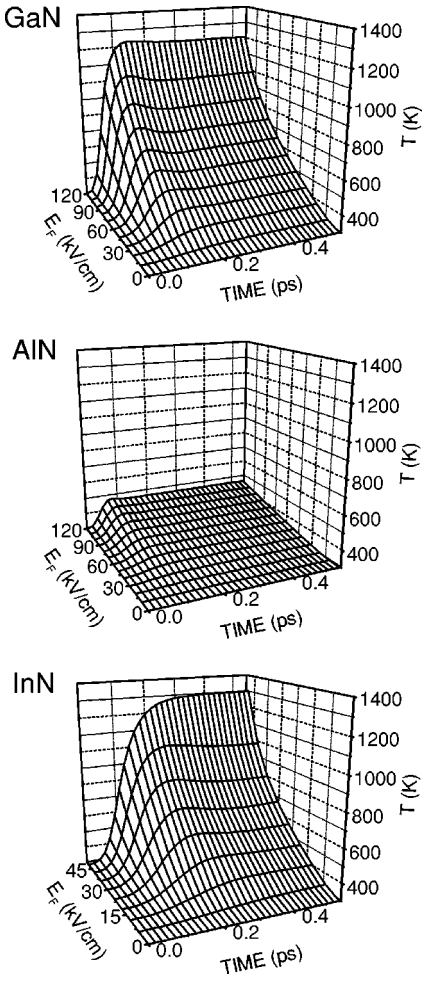


FIG. 2. Time evolution towards the steady state of the electron quasitemperature in GaN (upper figure), AlN (middle panel), and InN (lower figure).

field for the onset of the velocity overshoot in wurtzite AlN, GaN, and InN are much smaller than those obtained in the Monte Carlo simulations performed by Foutz *et al.*[16] This cannot be mostly due to the intervalley scattering they have considered (which is not effective when the electric field intensity is smaller than 120 kV/cm for GaN and AlN, and 60 kV/cm for InN) nor the Fermi-Dirac-like distribution function we have used (after 100 fs the distribution function becomes a Fermi-Dirac-like), but is principally related to the high values of the electron effective masses in the $L-M$ and K valleys they have assumed. In contrast to the smaller than 25% electron drift velocity overshoot we have demonstrated for electric fields smaller than 120 kV/cm, the intervalley scattering related overshoot effect as obtained by Foutz *et al.*[16] is more than 100% stronger. Consequently, in the case of electric fields smaller than 120 kV/cm (60 kV/cm), the possible contribution of the overshoot effect to the improvement of GaN,AlN (InN) nitride based heterojunction field effect transistors should also be very limited.[16]

In conclusion, we have presented a study on the transient transport characteristics of wurtzite GaN, AlN, and InN using quantum transport equations derived from the nonequilibrium statistical ensemble formalism. The existence of overshoot in both the electron drift velocity and quasitemperature (or mean energy) was demonstrated, whose onset occurs at 20 kV/cm in GaN, 60 kV/cm in AlN, and 10 kV/cm in InN. Instead of being associated with intervalley scattering as some authors argued, the overshoot effects in GaN, AlN (InN) for electric field intensities smaller than 120 kV/cm (60 kV/cm), as shown, is a result of the relation beteween the carriers' relaxation rate of momentum and energy: overshoot follows if during the evolution of the macroscopic state of the system, under the action of the electric field, the former is larger than the latter.

The authors would like to acknowledge partial financial support received from the Brazilian National Research Council (CNPq), the Brazilian Ministry of Planning (FINEP), and the Ceará and São Paulo States Research Agencies (FUNCAP; FAPESP).

[1] S. J. Pearson, articles in *GaN and Related Materials*, in the series Optoeletronic Properties of Semiconductors and Superlattices (Gordon and Breach, New York, 1997); S. Nakamura and G. Fasol, *The Blue Laser Diode* (Springer, Berlin, 1997); S. N. Mohammad and H. Morkoç, Prog. Quantum Electron. **20**, 361 (1996); I. Akasaki and H. Amano, Jpn. J. Appl. Phys., Part 1 **36**, 5393 (1997), and references therein.
[2] K. Moore and R. J. Trew, Mater. Res. Bull. **22**, 50 (1997); M. A. Khan, J. N. Kuznia, D. T. Olson, W. J. Schaff, J. W. Burm, and M. S. Shur, Appl. Phys. Lett. **65**, 1121 (1994); M. A. Khan, Q. Chen, J. W. Yang, M. S. Shur, B. T. Dermott, and J. A. Higgins, IEEE Electron Device Lett. **17**, 325 (1996); M. S. Shur and M. A. Khan, Mater. Res. Bull. **22**, 44 (1997); Q. Chen, J. W. Yang, R. Gaska, M. A. Khan, M. S. Shur, G. J. Sullivan, A. L. Sailor, J. A. Higgins, A. T. Ping, and I. Adesida, IEEE Electron Device Lett. **19**, 44 (1998).
[3] B. Gelmont, K. Kim, and M. Shur, J. Appl. Phys. **74**, 1818 (1993).
[4] N. S. Mansour, K. W. Kim, and M. A. Littlejohn, J. Appl. Phys. **77**, 2834 (1995).
[5] J. Kolník, I. H. Oğuzman, K. F. Brennan, R. Wang, P. P. Ruden, and Y. Wang, J. Appl. Phys. **78**, 1033 (1995).
[6] M. Shur, B. Gelmont, and M. A. Khan, J. Electron. Mater. **25**, 777 (1996).
[7] U. V. Bhapkar and M. S. Shur, J. Appl. Phys. **82**, 1649 (1997).
[8] S. Krishnamurthy, M. Van Schilfgaarde, and A. Sher, Appl. Phys. Lett. **71**, 1999 (1997).
[9] J. D. Albrecht, R. P. Wang, P. P. Ruden, M. Farahmand, and K. F. Brennan, J. Appl. Phys. **83**, 4777 (1998).
[10] J. D. Albrecht, R. P. Wang, P. P. Ruden, M. Farahmand, and K. F. Brennan, J. Appl. Phys. **83**, 1446 (1998).
[11] S. K. O'Leary, B. E. Foutz, M. S. Shur, U. V. Bhapkar, and L. F. Eastman, Solid State Commun. **105**, 621 (1998).
[12] S. K. O'Leary, B. E. Foutz, M. S. Shur, U. V. Bhapkar, and L. F. Eastman, J. Appl. Phys. **83**, 826 (1998).
[13] E. Bellotti, B. K. Doshi, K. Brennan, J. D. Albrecht, and P. P. Ruden, J. Appl. Phys. **85**, 916 (1999).
[14] B. E. Foutz, L. F. Eastman, U. V. Bhapkar, and M. S. Shur, Appl. Phys. Lett. **70**, 2849 (1997).
[15] E. W. S. Caetano, R. N. Costa Filho, V. N. Freire, and J. A. P. da Costa, Solid State Commun. **110**, 469 (1999).
[16] B. E. Foutz, S. K. O'Leary, M. S. Shur, and L. F. Eastman, J. Appl. Phys. **85**, 7727 (1999).
[17] L. Lauck, A. R. Vasconcellos, and R. Luzzi, Physica A **168**, 789 (1990); J. R. Madureira, A. R. Vasconcellos, R. Luzzi, and L. Lauck, Phys. Rev. E **57**, 3637 (1998); C. G. Rodrigues, Ph.D. Thesis, Universidade Estadual de Campinas, Campinas, SP, Brazil, 2000 (unpublished).
[18] D. N. Zubarev, V. Morosov, and Gerd Röpke, *Statistical Mechanics of Nonequilibrium Processes* (Akademie, Berlin, 1996 and 1997, respectively), Vols. 1 and 2; R. Luzzi and A. R. Vasconcellos, Fortschr. Phys./ Prog. Phys. **38**, 887 (1990); R. Luzzi, A. R. Vasconcellos, and J. G. Ramos, *Foundations of a Nonequilibrium Ensemble Formalism*, in the series Fundamental Theories of Physics (Kluwer, Dordrecht, forthcoming).
[19] R. Luzzi, A. R. Vasconcellos, and J. G. Ramos, *Statistical Foundations of Irreversible Thermodynamics*, in the series Texte zur Physik (Teubner, Leipzig, forthcoming).
[20] A. C. Algarte, A. R. Vasconcellos, and R. Luzzi, Phys. Status Solidi B **173**, 487 (1992).
[21] V. N. Freire, A. R. Vasconcellos, and R. Luzzi, Phys. Rev. B **39**, 13264 (1989).