

Hot phonon effects on high-field transport in GaN & AlN.

Angela Dyson, Daniel R. Naylor & Brian K. Ridley

Abstract— We have studied the effects of hot phonons on the high-field transport in GaN & AlN. The dynamics of the non-equilibrium electron-LO phonon system is studied via an ensemble Monte-Carlo code. We find that under steady-state conditions the hot-phonons cause the randomization of the electron momentum and increase their mean energy leading to diffusive heating. Average electron energies of three and two times those in the equilibrium phonon cases are found for GaN and AlN at applied fields of 100 kV/cm and 350 kV/cm respectively. The electron velocity is reduced compared to the case with equilibrium phonons at the lattice temperature. In the transient regime peak velocities reached at overshoot are reduced when non-equilibrium phonons are taken into account.

Index Terms— hot carriers, Monte Carlo methods.

I. INTRODUCTION

There have been a number of reports on the inclusion of hot-phonons into Monte-Carlo (MC) semiconductor transport codes and the resulting effects [1-6], and there has been a recent renewed interest in this topic due to the use of materials such as GaN and AlN in high power, high field devices. In such materials, as the longitudinal optical (LO) phonon energy is very large, it is possible to drive the phonon population far from equilibrium under normal operating conditions, affecting the transport characteristics of these materials. A previous study of GaN and AlN was performed by Foutz *et. al.* [7] however, hot-phonon effects were not included. Later work by Ramonas *et. al.* [8] included these effects, though their study was limited to applied electric fields up to 14 kV/cm. Recent work has proposed that hot electrons may be responsible for the degradation of AlGaIn/GaN & InAlN/GaN HFET's at larger applied fields [9], with electron temperatures measured experimentally at 2600 K and 5000 K respectively [10]. While such high temperatures may be highly localised it is clear that

Manuscript received April 16, 2015; revised August 3, 2015; accepted August 24, 2015. This work was supported by the Office of Naval Research under grant N00014-09-0777 & grant N00014-06-1-0267.

A. Dyson is with Department of Physics, University of Hull, Hull, HU6 7RX, UK (e-mail a.dyson@hull.ac.uk)

B. K. Ridley is with the School of Computer Science and Electronic Engineering, University of Essex, Wivenhoe Park, Colchester, Essex, CO43SQ, UK (e-mail: bkr@essex.ac.uk).

D. R. Naylor was with University of Hull, Hull, HU6 7RX, UK. He is now with Tessella.

Digital Object Identifier 10.1109/TED.2015.2476383

hot phonon effects cannot be neglected. Sophisticated MC codes that take account of these effects are usually coupled to Poisson solvers[4] and often isothermal or electro-thermal solvers[5,6]. Data from these codes tend to be published in the form of current voltage characteristics, results that are necessarily steady-state, and are therefore of little use in diagnosing the role of hot-electrons in device degradation. In this communication, we study the steady state and transient transport in GaN and AlN with a dynamic phonon distribution which is updated periodically.

II. METHOD

We have developed an ensemble bulk Monte-Carlo simulation in which hot phonons are included using the algorithm outlined by Jacaboni & Lugli [1], where the scattering and phonon occupation tables are updated every 25 fs. Details of the implementation with equilibrium phonons at the lattice temperature can be found elsewhere [11,12]. Material parameters for GaN and AlN are those from the wurtzite forms however we adopt the commonly used approximation that we have a single LO mode and we ignore the dispersion since it is small. It is also assumed that the lower gamma valley has a non-parabolic form and the equivalent upper valleys are parabolic. The scattering mechanisms considered are (1) ionised impurity, (2) polar optical phonon, (3) acoustic deformation potential, (4) intervalley and (5) piezoelectric. Screening and degeneracy effects are not currently included. The simulations are performed with 100,000 superparticles. The main parameters used in the model are given in table 1 and are from [5], with the exception of the valley separation in GaN which is taken from a recent experimental result [13] and is substantially lower than that employed by previous studies. The phonon lifetime is known to be a function of electron density and temperature in GaN [14] with measured lifetimes ranging between 2.5 ps and around 0.1 ps [15]. A phonon lifetime of 1 ps was chosen for both materials for ease of comparison. The lattice temperature is set to 300 K and the impurity concentration is set to 10^{17} cm⁻³ throughout.

III. RESULTS AND DISCUSSION

A. Steady-State

The results from the code including hot phonons are compared with those from equilibrium phonons. Figure 1 shows the velocity field characteristics. At low fields the difference is slight as expected; since the number of electrons capable of

(c) 2015 IEEE. Personal use of this material is permitted. Permission from IEEE must be obtained for all other users, including reprinting/ republishing this material for advertising or promotional purposes, creating new collective works for resale or redistribution to servers or lists, or reuse of any copyrighted components of this work in other works.

TABLE I
MATERIAL PARAMETERS

	GaN	AlN
Effective mass Γ valley	0.2	0.48
Effective mass upper valley	1.0	1.0
Optical phonon energy (meV)	91.2	99.2
Direct energy gap (eV)	3.39	6.2
Static dielectric constant	8.9	8.5
High frequency dielectric constant	5.35	4.6
Longitudinal sound velocity (10^3 m/s)	6.56	9.06
Transverse sound velocity (10^3 m/s)	2.68	3.70
Acoustic deformation potential (eV)	8.3	9.5
Valley separation, E_s (eV)	1.2	0.7;1.0
Piezoelectric constant e_{14} ($C.m^{-2}$)	0.375	0.92
Optical Phonon lifetime (ps)	1	1

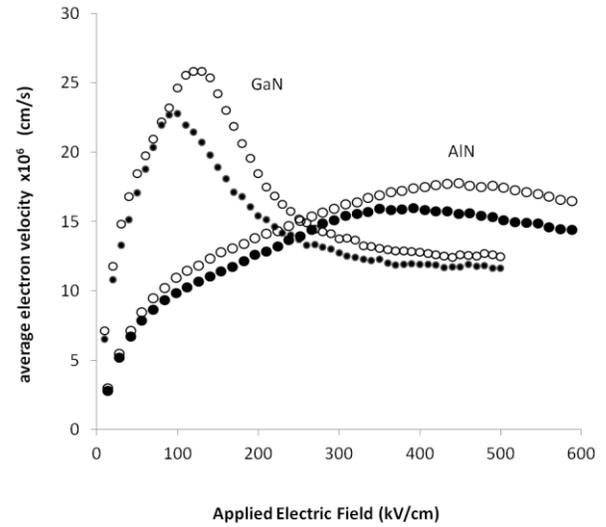


Fig. 1 – Steady-state velocity-field curve with equilibrium phonons open circles and with non-equilibrium phonons filled circles.

TABLE 2
CRITICAL FIELDS (kV/cm)

	GaN	AlN
With equilibrium phonons	130	450
With non-equilibrium phonons	100	350

emitting a phonon is small, the phonon population is not too different from thermal (see fig 2). The peak velocity is lower in the hot phonon case; as is the critical field. For GaN we find peak velocities of 2.6×10^7 cm/s and 2.3×10^7 cm/s at applied electric fields of 130 kV/cm and 100 kV/cm, while for AlN we find peak velocities of 1.8×10^7 cm/s and 1.6×10^7 cm/s at applied electric fields of 450 kV/cm and 350 kV/cm. This data is collected in table 2. The equilibrium phonon results for AlN are identical to results of [7] while for GaN the slight differences presumably originate in the intervalley separation being lower in our simulation. Foutz *et. al.* find a peak velocity of 2.9×10^7 cm/s at a critical field of 140 kV/cm for GaN. Barker *et. al.* measured peak velocities between 2.0×10^7 and 2.5×10^7 cm/s at critical fields between 130 and 180 kV/cm in four samples [16]. The critical field and peak velocities are particularly sensitive to the valley separation as described previously [11].

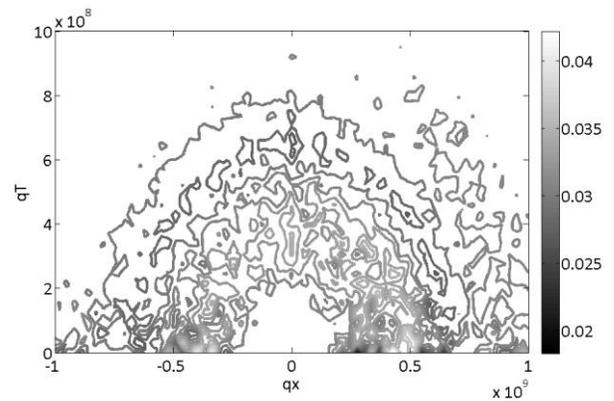


Fig. 2 – Non-equilibrium phonon population as a function of phonon wave vector for an applied field of 10 kV/cm for GaN, where q_x is the phonon wavevector component in the direction of the applied field and q_T is the component in the plane.

(c) 2015 IEEE. Personal use of this material is permitted. Permission from IEEE must be obtained for all other users, including reprinting/ republishing this material for advertising or promotional purposes, creating new collective works for resale or redistribution to servers or lists, or reuse of any copyrighted components of this work in other works.

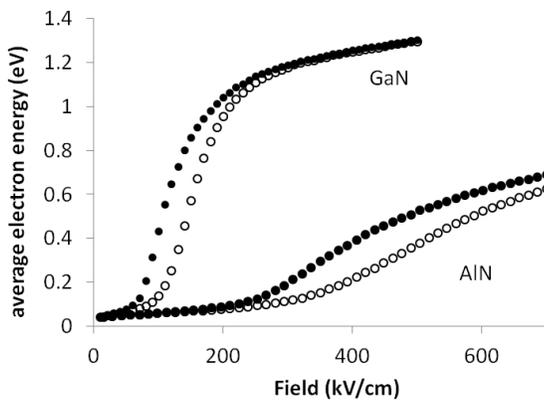


Fig. 3 – Average electron energy as a function of applied field; with equilibrium phonons open circles and with non-equilibrium phonons filled circles.

We can see in Figure 3 that the average energy is greater with hot phonons enabled for fields between 60 and 300 kV/cm for GaN and beyond 200 kV/cm for AlN. For GaN the average energy is three times that found with equilibrium phonons at a field of 100 kV/cm; while for AlN it is twice that with equilibrium phonons at a field of 350 kV/cm. Figure 4 shows the number of superparticles used in the simulation as a function of their average energy at an applied field of 60 kV/cm. The energy peak with equilibrium phonons corresponds to thermal energy. With non-equilibrium phonons enabled there are more electrons at higher energies and fewer at thermal. These results are of particular significance for the formation of defects and the subsequent device degradation. A recent study applying the results from a 2D Poisson and drift-diffusion model to an ensemble Monte-Carlo method with equilibrium phonons predicted an average energy of 1.5 eV with a substantial tail extending to over 3 eV [17]. The electrons are confined with concomitant higher mobility than our bulk code but our results would suggest that if hot phonons were taken into account the energies would be higher.

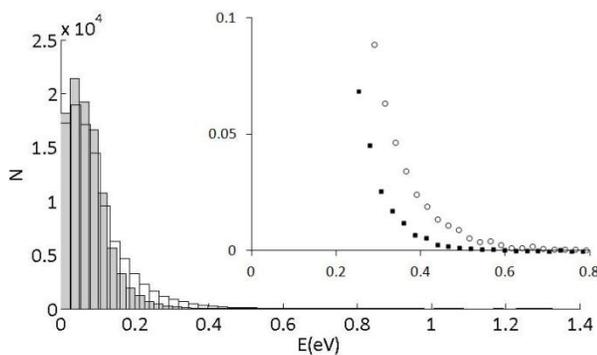


Fig. 4 – Histogram showing superparticle number as a function of their average energy; with equilibrium phonons grey bars and with non-equilibrium phonons white bars. Inset with the data extracted from the histogram but with reduced scale on both axes. GaN with an applied field of 60 kV/cm.

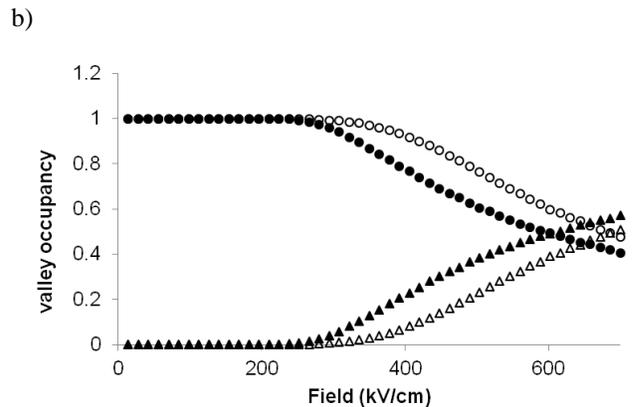
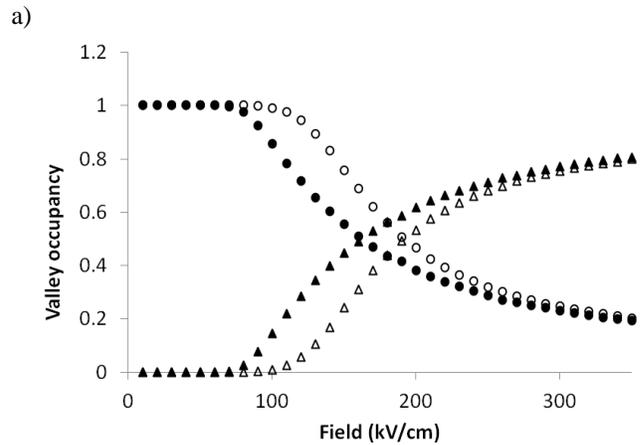


Fig. 5 - Valley occupancy as a function of applied field; with equilibrium phonons open markers and with non-equilibrium phonons filled markers. a) GaN & b) AlN

With higher average energies in the non-equilibrium phonon case it is possible for electrons to make an intervalley transfer at a lower field than is the case with phonons at the lattice temperature. Hence the critical field is lower with non-equilibrium phonons, the effect of which can be identified by examining the valley occupancy, as shown in figure 5. With hot phonons enabled electrons transfer to the upper valleys at a field of 70 kV/cm (210 kV/cm) while without hot phonons the onset occurs at 90 kV/cm (250 kV/cm). Therefore in the hot phonon case the energy is higher while the velocity is lower, we attribute this to diffusive heating.

Figure 6 shows how the polar-optical phonon scattering rate evolves as the phonon population is driven away from equilibrium. The applied field is 50 kV/cm for GaN and 182 kV/cm for AlN. The rates are shown at the start of the simulation and at 1 and 4 ps into the simulation. Even at these modest fields of around half the critical field, the absorption rate increases by almost an order of magnitude for GaN and by 5 times for AlN. It is this increased re-absorption rate that increases the electron energy.

a)

(c) 2015 IEEE. Personal use of this material is permitted. Permission from IEEE must be obtained for all other users, including reprinting/ republishing this material for advertising or promotional purposes, creating new collective works for resale or redistribution to servers or lists, or reuse of any copyrighted components of this work in other works.

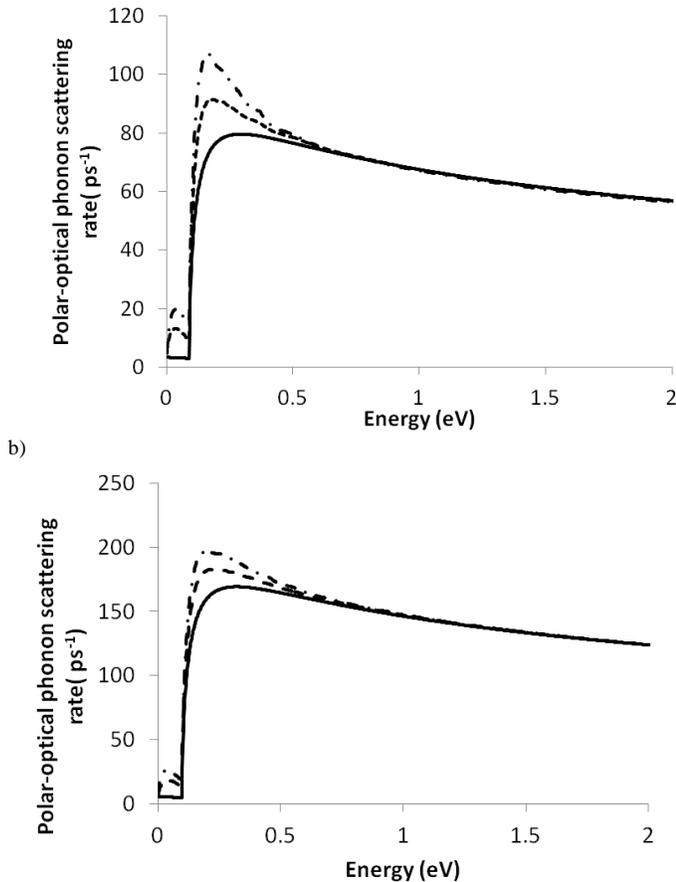


Fig. 6 - Polar-optical phonon scattering rate as a function of energy at simulation times of 0 (solid line), 1 (dash line) & 4 ps (chain line) for a) GaN at 50 kV/cm b) AlN at 182 kV/cm .

The energy relaxation time as a function of average electron energy is shown in figure 7. The energy relaxation time is calculated using equation 1 [18] where E is the average electron energy, E_0 is the energy at the lattice temperature and $F(E)$ and $v[F(E)]$ are the energy dependent field and electron velocities taken from the steady state results. At low energies most of the electrons have insufficient energy to emit an optical phonon and the energy relaxation time is long. Energy relaxation times are longer with non-equilibrium phonons enabled. The energy relaxation times are 2.6×10^{-13} s and 5.6×10^{-14} s for GaN and AlN respectively with equilibrium phonons. Our AlN value is identical to [7] but for GaN they find 3.5×10^{-13} s, which is slightly larger than our 2.6×10^{-13} s ; again the differences are presumably down to the intervalley separation being smaller in our case. With non-equilibrium phonons included our values become 3.2×10^{-13} s for GaN and 6.9×10^{-14} s for AlN.

The energy relaxation time gives an indication of transient effects. We would therefore expect transient effects to be weaker in AlN than GaN because the relaxation time is longer in GaN. We also expect that the inclusion of non-equilibrium phonons would enhance the transient effects due to the increase in energy relaxation time.

$$\tau_E = \frac{E - E_0}{q \langle F(E) v[F(E)] \rangle} \quad (1)$$

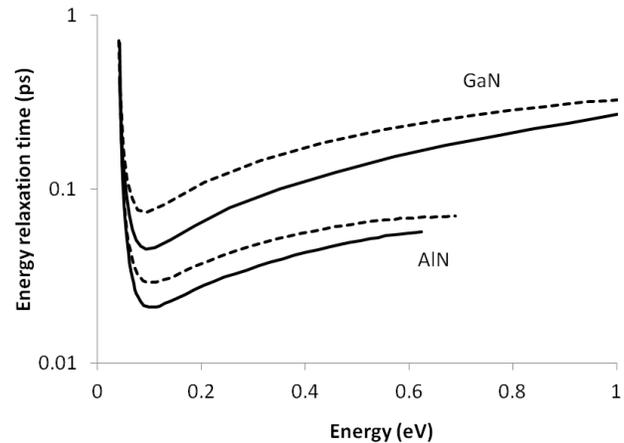


Fig. 7 - Energy relaxation time as a function of average electron energy in eV. Equilibrium phonons solid line and with non-equilibrium phonons dash line; upper lines GaN lower AlN.

B. Transient

In figure 8 we plot the average velocity of electrons in GaN with non-equilibrium phonons as a function of simulation time. Velocity overshoot appears with applied fields above 100 kV/cm; this is the same as the steady-state critical field i.e. the field at which the peak steady-state velocity occurs. As the field is increased the peak velocity reached at overshoot increases but the duration of the overshoot decreases. There is

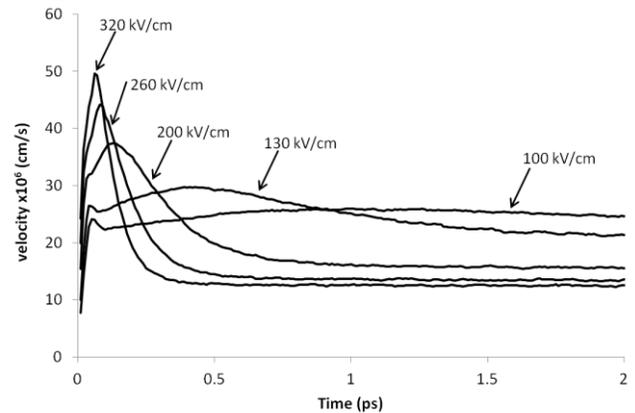


Fig. 8 - Velocity-time curves with non-equilibrium phonons in GaN at applied fields of 100, 130, 200, 260 & 320 kV/cm.

a small shoulder to the curves at very early times; between 50 - 100 fs. At 50 fs the average electron energy just reaches the threshold for emission of an optical phonon; the momentum change experienced by the electron results in a reduction in velocity. We therefore attribute this shoulder to the onset of

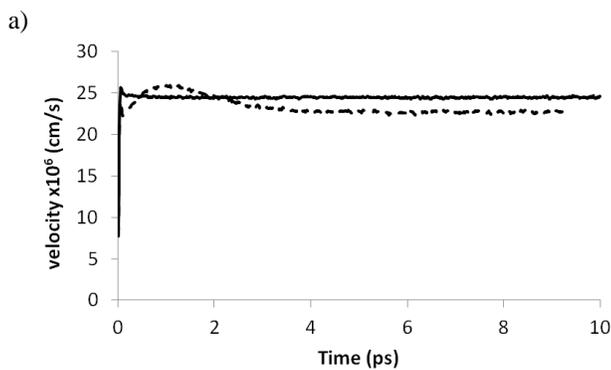
(c) 2015 IEEE. Personal use of this material is permitted. Permission from IEEE must be obtained for all other users, including reprinting/ republishing this material for advertising or promotional purposes, creating new collective works for resale or redistribution to servers or lists, or reuse of any copyrighted components of this work in other works.

polar optical phonon emission. Wraback *et. al.* have measured transient electron velocities [19]. At an applied field of 130 kV/cm they find a peak velocity of 3.5×10^7 cm/s while our non-equilibrium phonon result gives 3.0×10^7 cm/s.

The remainder of the transient results are presented in two ways, either by comparison of equilibrium and non-equilibrium phonons at the same applied field or at an applied field which is the same fraction of the critical field.

We begin by comparing equilibrium and non-equilibrium phonon results at the same applied field; 100 kV/cm for GaN and 336 kV/cm for AlN. These values were chosen to highlight the effects of a shift in the critical field because the relaxation of velocity overshoot is directly correlated with intervalley transfer [7]. Figure 9 shows the electron velocity as a function of time. There is a clear velocity overshoot in the non-equilibrium phonon curves. This is because the steady-state critical fields with non-equilibrium phonons and equilibrium phonons are different. This is particularly noticeable in GaN at an applied field of 100 kV/cm (figure 9a), the simulation with non-equilibrium phonons has entered a regime of velocity overshoot while that with equilibrium phonons has not. We also see that in GaN, a portion of the curve exceeds the equilibrium phonon result albeit for a very short time whilst in AlN the velocities remain lower with hot phonons enabled at all fields..

Figure 10 shows the non-equilibrium phonon distribution at an applied field of 100 kV/cm. Recall that figure 2 demonstrated that at a low applied field (10 kV/cm) the phonon distribution does not differ very much from equilibrium and, by comparison with figure 10, it is clear that at higher applied fields the phonon distribution becomes shifted in momentum space, reflecting the dominance of forward phonon scattering. This phonon redistribution in momentum space was also observed in GaAs by [3]. The distribution also deviates significantly from equilibrium. The broad phonon spectrum leads to a randomization of electron momentum and



b)

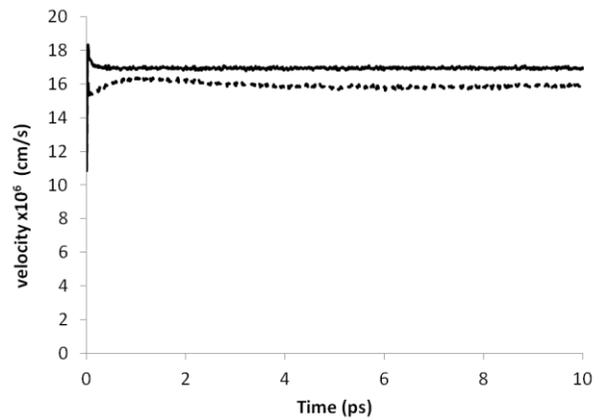


Fig. 9 - Velocity-time curve with equilibrium phonons solid line and with non-equilibrium phonons dash line. Applied field is a) 100 kV/cm for GaN and b) 336 kV/cm for AlN.

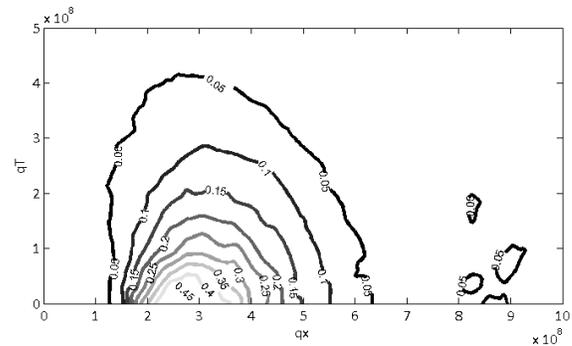


Fig 10 - Non-equilibrium phonon population as a function of phonon wave vector for an applied field of 100 kV/cm in GaN at 0.1 ps.

is the origin of the reduced velocity in the non-equilibrium phonon case.

In light of the steady-state critical field differences it is instructive to compare the transient results at fields which are the same fraction of the steady-state critical field of the respective materials, rather than the same absolute applied fields. Figure 11 shows the velocity overshoot in both materials for fields corresponding to twice the critical field. The fields for each curve in figure 11 are listed in table 3. Our results with equilibrium phonons are similar to [7], slight differences are presumably due to the smaller intervalley separation in our simulation. The overshoot appears to be

TABLE 3
OVERSHOOT FIELDS (kV/cm)

	GaN	AlN
With equilibrium phonons	260	896
With non-equilibrium phonons	200	700

(c) 2015 IEEE. Personal use of this material is permitted. Permission from IEEE must be obtained for all other users, including reprinting/ republishing this material for advertising or promotional purposes, creating new collective works for resale or redistribution to servers or lists, or reuse of any copyrighted components of this work in other works.

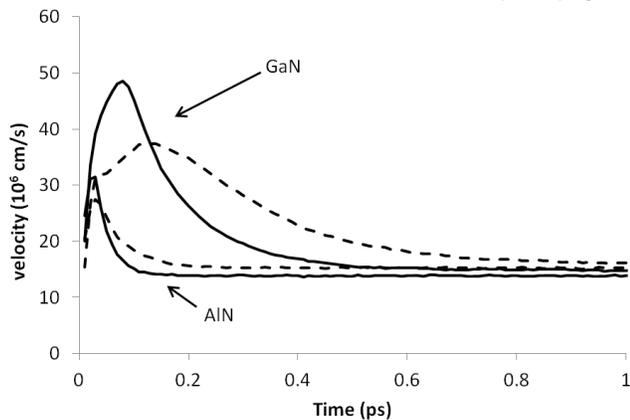


Fig 11 - A comparison of velocity overshoot in GaN and AlN with equilibrium phonons (solid lines) and non-equilibrium phonons (dash lines). Applied field is twice critical in each case.

prolonged in GaN, this is due to the higher field required for the equilibrium phonon case. As already described the duration of the velocity overshoot decreases as the applied field is increased. The effect of the non-equilibrium phonons is to reduce the peak velocity reached in both materials; already identified as due to the randomization of electron momentum which is caused by the broad phonon spectrum.

III. CONCLUSIONS

We have studied the effects of non-equilibrium phonons on the high-field transport in GaN and AlN, paying particular attention to the evolution of the phonon distribution. We find that under steady-state conditions the hot-phonons cause the randomization of the electron momentum and increase their mean energy leading to diffusive heating. For GaN (AlN) the average energy of the electrons is three (two) times that of the equilibrium phonon case at an applied field of 100 kV/cm (350 kV/cm). These results imply that high electron energies predicted by simulations with equilibrium phonons are underestimates and that the diffusive heating leads to a reduction in the steady-state critical field and an increase in the energy relaxation time. In the transient regime, peak velocities reached at overshoot increase as the applied field is increased. The duration of the overshoot is reduced as the applied field increases. Overshoot velocities are reduced in the case where non-equilibrium phonons are considered.

ACKNOWLEDGMENT

This work was supported by the Office of Naval Research sponsored by Dr. Paul Maki grant nos. N00014-09-1-0777 & N00014-06-1-0267.

REFERENCES

- [1] P. Lugli, C. Jacoboni, L. Reggiani and P. Kocevar, "Monte Carlo algorithm for hot phonons in polar semiconductors", *Appl. Phys. Lett.* vol. 50, 1251, 1987.
- [2] R. Mickevicius and R. Reklaitis, "Monte carlo study of nonequilibrium phonon effects in GaAs", *Solid State Comms.* vol. 64, pp1305-1308, 1987.
- [3] R. Mickevicius and R. Reklaitis, "Hot phonon effects on electron high-field transport in GaAs", *J Phys. C* vol. 1, pp9401-9412, 1989.
- [4] B. Padmanabhan, D. Vasileska & S. M. Goodnick *J. Comput Electron* vol. 11, pp129-136, 2012.
- [5] T. Sadi, R. Kelsall & N. Pilgrim, "Simulation of electron transport in InGaAs/AlGaAs HEMTs using an electrothermal monte carlo method", *IEEE Trans. Elect. Devices*, vol. 53, 2006.
- [6] T. Sadi & R. Kelsall, "Hot-phonon effect on the electrothermal behavior of submicrometer III-V HEMTs", *IEEE Trans. Elect. Devices* vol. 28, 2007.
- [7] B. E. Foutz, S. K. O'Leary, M. S. Shur and L. F. Eastman, "Transient electron transport in wurtzite GaN, InN and AlN", *J. Appl. Phys.* vol. 85, 7727, 1999.
- [8] M. Ramonas, A. Matulionis & L. Rota "Monte-Carlo simulation of hot-phonon and degeneracy effects in the AlGaIn/GaN two-dimensional electron gas channel", *Semicond. Sci. Technol.* vol. 18, pp118-123, 2003.
- [9] C. Y. Zhu *et al.*, "Degradation and phase noise of InAlN/AlN/GaN heterojunction field effect transistors: Implications for hot electron/phonon effects", *Appl. Phys. Lett.*, vol. 101, 103502, 2012.
- [10] M. Tapajna *et al.* "Hot-electron-related degradation in InAlN/GaN high-electron-mobility transistors" *IEEE Trans. Electron. Devices.* vol. 61, 2793, 2014
- [11] D. R. Naylor, A. Dyson & B. K. Ridley, "Steady-state and transient electron transport in bulk GaN employing an analytic bandstructure", *Solid State Comm.* vol. 152, pp549-551, 2012.
- [12] D. R. Naylor, A. Dyson & B. K. Ridley, "Steady-state and transient electron transport properties of bulk dilute GaN_xAs_{x-1}", *J. Appl. Phys.* vol. 111, 053703, 2012.
- [13] M. Semenenko, O. Yilmazoglu, H. L. Hartnagel, D. Pavlidis, *J. Appl. Phys.* vol. 109, 023703, 2011.
- [14] A. Dyson & B.K. Ridley, "Hot phonon plasmon modes in GaN", *J. Appl. Phys.* vol. 108, 104504, 2010.
- [15] J. H. Leach *et al.* "Degradation in InAlN/GaN- based heterostructure field effect transistors: Role of hot phonons", *Appl Phys. Lett.* vol. 95, 223504, 2009.
- [16] J. M. Barker *et al.*, "High-field transport studies of GaN", *Physica B* vol 314, 39-41, 2002.
- [17] Y. Puzryev *et al.* "Gate bias dependence of defect-mediated hot-carrier degradation in GaN HEMTs", *IEEE Trans. Electron. Devices.* vol. 16, 1316, 2014.
- [18] M. Shur "Physics of semiconductor devices" Solid state physical electronics series ed. N. Holonyak Jr., Prentice Hall, 1990.
- [19] M. Wraback *et al.*, "Direction dependent band nonparabolicity effects on high-field transient electron transport in GaN", *Appl. Phys. Lett.*, vol 82, 3674, 2003.

Angela Dyson received the BSc (Honors) degree in theoretical physics and the PhD degree in theoretical plasma physics from the University of Essex, Colchester, UK, in 1994 and 1999 respectively. Since 2007 she has been a Lecturer in the Department of Physics at the University of Hull; where she was promoted to senior lecturer in 2013. She has worked in the area of semiconductor device theory and modeling for 11 years. Her current research interests include high field transport, monte carlo device simulation and compact sources of terahertz radiation.

Daniel R. Naylor received the B.Sc. degree (Honors) in physics, in 2008, and the Ph.D. degree in 2012, both from the University of Hull, U.K. In 2013, he joined Tessella.

Brian K. Ridley received the BSc (Honors) degree and the Ph.D. from the University of Durham, U.K. He was at The Mullard Research laboratory from 1956-1964. He joined the University of Essex in 1964 where he was promoted to Professor in 1984. He has held visiting Professorships at many learned institutions over the years e.g. Princeton, Lund, Santa Barbara and Cornell. He has authored many books including "Time, Space and Things" which has been translated into 7 languages and "Quantum Processes in Semiconductors" now in its 5th edition. His research interests include the Ridley-Watkins-Hilsum effect, N.D.R. domains and filaments, hot electrons, scattering and trapping mechanisms, the acoustoelectric effect, the physics of low-dimensional systems, elasticity theory of optical phonons, quantum confinement of optical

(c) 2015 IEEE. Personal use of this material is permitted. Permission from IEEE must be obtained for all other users, including reprinting/ republishing this material for advertising or promotional purposes, creating new collective works for resale or redistribution to servers or lists, or reuse of any copyrighted components of this work in other works.

phonons, impact ionization and breakdown, large-bandgap semiconductors, especially the III-V nitrides, hot phonons, spin relaxation & THz generation.