Low-temperature diffusion thermopower in GaN/AlGaN heterojunctions: Effect of dislocations

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The diffusion thermopower S_d of the two-dimensional electron gas at a GaN/AlGaN heterojunction is studied, in detail, in the low-temperature region $T<30$ K. The important mechanisms of scattering of electrons considered are those by edge dislocations, remote and background impurities, interface charges and roughness, and bulk acoustic phonons via deformation potential and piezoelectric fields. The dominant contribution to S_d is found to be from dislocations via the coulomb interaction; the contribution from strain field associated with the dislocations is, comparatively, small. The contribution from acoustic phonons is negligible. The calculations, for pure samples without dislocations in the low-temperature region where acoustic phonon scattering dominates, bring out the characteristics of the Bloch-Grüneisen regime, as in mobility studies.

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I. INTRODUCTION

Over the past few years, GaN due to its direct, large band gap has attracted attention as a potential material system for use in high-power, high-frequency, high-temperature applications, such as blue and UV light-emitting devices, laser diodes, and HEMTs.[1–3] The performance of the electronic devices based on GaN/AlGaN modulation doped heterostructure is, to a large extent, determined by the transport properties of the two-dimensional electron gas (2DEG) confined at the GaN/AlGaN interface. Investigations of mobility have been made[4–10] to assess the relative importance of the different scattering mechanisms operative in both zinc-blende (ZB) and wurtzite (WZ) structures of GaN. The low-temperature electron mobility is found to be limited by impurities, interface roughness, alloy-disorder, dislocations, and acoustic phonons, with dislocation scattering being the major contributor.[6] In recent years, the study of the effect of dislocations on transport in a 2DEG at GaN/AlGaN modulation doped heterostructures has attracted a lot of attention.[6–14] The epitaxial layers of GaN are most commonly grown on sapphire or SiC substrates. The large lattice and thermal mismatch between the epitaxial layer and the substrate material leads to a high density (typically 10^8–10^{10} cm^{-2}) of dislocations.[7,11,15] TEM investigations of GaN/AlGaN HEMT structures have shown that threading dislocations originate at the substrate-buffer interface and propagate to the sample surface. Their line is roughly parallel to the *c* axis and the large majority are edge type passing through the 2DEG; the screw dislocations near the substrate-buffer interface decrease with distance.[8,11] The transport properties of the 2DEG device will, therefore, be strongly influenced by the edge dislocations.

Thermopower is an important transport property, sensitive to the composition and structure of a system and to the external fields. Diffusion thermopower reflects the energy dependence of a scattering mechanism and is determined not only by the magnitude of the scattering, but also by details concerning the distribution of the scatterers and their type. It is, therefore, a sensitive probe of the dominant scattering mechanisms in a system. Thermopower has been studied, both experimentally and theoretically, in detail, in low-dimensional semiconductor systems, particularly of GaAs/AlGaAs.[16–18] However, there exist very few investigations of this interesting property in the case of GaN/AlGaN system, which, unlike GaAs, is distinguished by the presence of dislocations.

The purpose of the paper is twofold: First, to illustrate the importance of dislocation scattering, in thermopower studies, as compared to the other scattering mechanisms in 2DEG systems; and second, to present detailed calculations of the low-temperature diffusion thermopower S_d of 2DEG at a HJ of the representative material system GaN/AlGaN, where dislocations are important. The outline of the paper is as follows. In Sec. II, the theory describing electron diffusion thermopower is given. Besides the expression for S_d, the details of the various scattering mechanisms contributing to S_d are also given. Expressions for the relaxation rates for dislocation scattering incorporating the finite extent of the 2DEG have been developed. In Sec. III, the results of the detailed numerical calculations are presented and discussed. We show that the dominant contribution to S_d is from dislocations via the coulomb interaction, the contribution from strain field associated with the dislocations being comparatively small. In the low-temperature region, for pure samples, the characteristics of the Bloch-Gruneisen regime are noticed, for the first time, in thermopower, as in mobility studies. Conclusions are given in Sec. IV.

II. THEORY

A. Wave functions and eigenvalues

We consider a 2DEG spatially confined along *z* direction perpendicular to the interface in a GaN/AlGaN HJ with $z>0$ on the GaN side. The electron wave function and the energy eigenvalues are given by[19]

$$\psi_n(\mathbf{r},z) = \xi_n(z)e^{ik.\mathbf{r}} \tag{1}$$

and

$$E_n(\mathbf{k}) = E_n + \frac{\hbar^2 k^2}{2m^*}, \tag{2}$$

where $\mathbf{r}=(x,y)$ and $\mathbf{k}=(k_x,k_y)$ are the 2D position and wave vectors of an electron with effective mass m^* and $\xi_n(z)$ is the normalized wave function of the nth electric subband with energy E_n associated with it. We will, in what follows, assume that the electrons in the inversion layer occupy only the lowest subband $(n=0)$ and that the confinement profile is described by Fang-Howard variational wave function,[19]

$$\xi_o(z) = \left(\frac{b^3 z^2}{2}\right)^{1/2} \exp(-bz/2), \tag{3}$$

with b, the variational parameter, given by

$$b = \left[\frac{48\pi m^* e^2}{\kappa_s \hbar^2}\right]^{1/3} \left(n_{\text{depl}} + \frac{11}{32} n_s\right)^{1/3}. \tag{4}$$

Here, κ_s is the static dielectric constant, n_s is the 2D electron concentration in the inversion layer, and n_{depl} is the depletion layer concentration.

B. Diffusion thermopower

Thermopower S is defined by the relation,[16]

$$\mathbf{E} = S\,\boldsymbol{\nabla} T \tag{5}$$

under open circuit conditions, where $\mathbf{E}$ is the effective electric field produced by the temperature gradient $\boldsymbol{\nabla} T$. In the presence of temperature gradient, the carriers diffuse through the specimen interacting with a random distribution of scattering centers. The heat flux carried by the carriers yields the diffusion thermopower S_d. In addition, the induced phonon momentum current drags electrons with it as a result of electron-phonon interaction to produce the phonon-drag contribution S_g. Employing the Boltzmann transport formalism, with $\boldsymbol{\nabla} T$ in the plane of the 2DEG, the diffusion contribution to thermopower, S_d, in the relaxation time approximation, is given by[17]

$$S_d = \left(\frac{1}{eT}\right)\left[-E_F + \left(\frac{\langle E\tau(E)\rangle}{\langle \tau(E)\rangle}\right)\right] \tag{6}$$

with

$$\langle F(E)\rangle = \frac{\int F(E)E(-\partial f_o/\partial E)dE}{\int E(-\partial f_o/\partial E)dE}. \tag{7}$$

Here $\tau(E)$ is the relaxation time of the electrons, $f_o(E)$ is the Fermi-Dirac distribution function and E_F is the Fermi energy determined by the electron concentration. Eq. (6) can be used to evaluate S_d for the various scattering mechanisms. The total S_d can be calculated assuming the overall relaxation time τ to be given by Matthiessen's rule:[20] $\tau^{-1}=\Sigma_i \tau_i^{-1}$.

Often we find in literature limiting forms of S_d being used in the analysis of data. In the degenerate limit, a good approximation to Eq. (6) is the well-known Mott expression[16]

$$S_d = \frac{\pi^2 k_B^2 T}{3e}\left[\frac{d}{dE}\ln(\sigma(E))\right]_{E=E_F}, \tag{8}$$

where $\sigma(E)$ is the energy dependent conductivity. If the energy dependence of the relaxation time is taken as E^p, Eq. (8) can be more simply expressed as[18,21]

$$S_d = \frac{\pi^2 k_B^2 T}{3eE_F}(p+1), \tag{9}$$

where the first term reflects the scattering mechanisms. The parameter p can be expressed in the form[21] $p=[d\ln(\tau(E))/dE]_{E=E_F}$, thus bringing out the feature that S_d is determined not only by the magnitude of the scattering but also the energy dependence of $\tau(E)$ at $E=E_F$. In this paper we employ, in our calculations, the complete expression [Eq. (6)], without any approximations.

C. Scattering mechanisms

Here, we describe the various scattering mechanisms influencing diffusion thermopower. The dominant scattering mechanisms operative in the 2DEG at a HJ are now well established and their scattering theories well developed.[19,22] In the low-temperature ($T<30$ K) region of interest, the electrons in the inversion layer are considered to be scattered by remote impurities (RIs), background impurities (BIs), interface roughness (IFR), interface charges (IFC), and bulk acoustic phonons via deformation potential (DP) and piezoelectric (PZ) couplings. With a view to study the effect of dislocations on S_d, we also assume the electrons to be scattered by dislocations via coulomb (DC) and strain fields (DS). The influence of alloy disorder in the AlGaN barrier layer on 2DEG is neglected; the wave function [Eq. (3)] vanishes at the interface. The inherent piezoelectric property of nitrides induces a high-density 2DEG ($n_s \sim 10^{12}-10^{13}$ cm^{-2}) at the HJ. For simplicity, we assume that screening is essentially static and is determined solely by electrons in the lowest subband.

1. Dislocation scattering

In a GaN/AlGaN heterostructure, the number and orientation of the dislocations in the GaN layers is strongly dependent on factors, such as the sample preparation conditions, the layer thickness, and the magnitude of lattice mismatch.[1–3,8] We restrict ourselves to WZ GaN and picture-edge dislocations to be oriented parallel to the c axis, the conventional growth direction of WZ GaN, and to thread through the interface between the GaN layer and AlGaN layer.[8–12,23] Edge dislocations produce two types of scattering potentials affecting the 2DEG. One is the Coulomb potential produced by the charges on the dislocation lines. The other mechanism responsible for scattering is the long-range strain field surrounding the dislocation lines via deformation and piezoelectric potentials; in GaN, the dislocations parallel to the c axis do not couple any piezoelectric potential.[23,24]

Most recent investigations of the low-field transport of GaN have been made in the frame of the relaxation time concept.[7–14] Jena and co-workers,[12,14] with a view to under-

stand transport in GaN/AlGaN HEMTs, developed a theory of electron scattering by edge dislocations threading a perfect degenerate 2DEG and identified dislocation scattering as a mobility-limiting scattering mechanism. Following the treatment given by Jena *et al.*[12] for charged dislocation scattering in a perfect 2DEG at a HJ, we have extended the formalism for the relaxation time to include the finite extent of the 2DEG along the *z*-direction. Considering a dislocation as a line of charge with charge density ρ_L threading through the quasi-2DEG and using the screened potential, modified to include the finite extent of the 2DEG,[19] we obtain the following expression for the relaxation time:

$$\tau_{\mathrm{DC}}^{-1} = \frac{2\pi e^2 m^* \rho_L N_{\mathrm{dis}}}{\hbar^3 \kappa_s^2 k^3} \int_0^{2k} dq \frac{|A(q)|^2}{\varepsilon^2(q)} \frac{1}{\sqrt{1 - q^2/4k^2}} \tag{10}$$

where

$$A(q) = \begin{cases} \dfrac{b^3}{(b+q)^3 q} + \dfrac{b^3 - a_0 b^2 q - a_1 b q - 2a_2 q}{(b-q)^3}, & q \neq b \\ \dfrac{b^3}{(b+q)^3 q} + \dfrac{15}{8b}, & q = b \end{cases} \tag{11}$$

with $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ and the expressions for a_0, a_1 and a_2, are given by Ando *et al.*[19] In Eq. (10), N_{dis} is the 2D dislocation density, and ρ_L is, to a very good approximation, given by ef/c_o, c_o being the lattice constant in the (0001) direction of WZ GaN and f the fraction of filled acceptor states.[12]

Allowing for the inclusion of the envelop function along the perpendicular *z* direction and considering the scattering of the electrons from the strain fields surrounding edge dislocations, via screened deformation potential interaction, Joshi *et al.*[6] have obtained an analytical expression for the scattering rate. By weighting the integrand in the expression for the scattering rate with factor $q^2/2k^2$, we obtain the relaxation time:

$$\tau_{\mathrm{DS}}^{-1} = \frac{a_c^2 b_e^2 m^* N_{\mathrm{dis}}}{2\pi\hbar^3 k^3 \kappa_s^2} \left(\frac{1-2\gamma}{1-\gamma}\right)^2 \int_0^{2k} dq \frac{(1 + 84.3q^2/8b^2)}{\varepsilon^2(q)\sqrt{1-(q/2k)^2}}. \tag{12}$$

Here, a_c is the conduction band deformation potential, b_e is the magnitude of the Burger's vector of the edge dislocations, and γ is the Poisson ratio for the crystal.

For the low temperatures considered, we use in Eqs. (10) and (12), the following expression for the screening function:

$$\varepsilon(q) = 1 + \frac{2\pi e^2}{\kappa_s q} F(q)\Pi(q) \tag{13}$$

where $F(q) = 8 + 9w + 3w^2/8(1+w)^3$, with $w = q/b$, is the form factor for electron-electron interaction[19] and the static polarizability function is taken to be $\Pi(q) = m^*/\pi\hbar^2$.

2. Impurity scattering

In modulation-doped HJ systems, the scattering of the carriers by impurities can arise from the BI in the GaN layer and the RI in the AlGaN barrier layer as well as the charges at the GaN/AlGaN interface. The relaxation times for these three distributions of impurities have been worked out by Walukeiwicz *et al.*[22] using the approach of Ando *et al.*[19] Considering the scattering by the ionized donors in the AlGaN layer to be caused by the fluctuations in the average field of the donors and not by their distribution itself,[25,26] the relaxation time in the case of RIs is

$$\tau_{\mathrm{RI}}^{-1} = C_0 \frac{b^6 N_{\mathrm{RI}}^{1/3}}{6k^2} \int_0^{2k} dq \frac{q^3}{P_o(q,b)(4k^2 - q^2)^{1/2}}, \tag{14}$$

where $C_0 = 128\pi m^* e^4/\hbar^3\kappa_s^2$, $P_o(q,b) = [8q(q+b)^3 + q_s(8b^3 + 9b^2 q + 3bq^2)]^2$ with $q_s = (2\pi e^2 n_s/\kappa_s k_B T\{[1 + \exp(-E_F/k_B T)].\ln[1 + \exp[E_F/k_B T]]\}^{-1}$ and N_{RI} is remote impurity concentration. It may be noted that the screening of the interaction appears in the factor $P_o(q,b)$.

In the case of BIs, scattering by the impurities in the GaN layer depends on the confinement of carriers and is important for HJ samples with thick barriers and/or wide spacer layers.[25,26] Using the approach of Ando *et al.*,[19] the relaxation time is given by[22]

$$\tau_{\mathrm{BI}}^{-1} = \frac{4C_0 N_{\mathrm{BI}}}{bk^2} \int_{0.5-x_k}^{0.5} dx \frac{F(x)(1-2x)}{[x_k^2 - (0.5-x)^2]^{1/2}}, \tag{15}$$

where $F(x) = 69 - 336x + 630x^2 - 580x^3 + 264x^4 - 48x^5/[32(1-2x)(1-x)^3 + \beta(10 - 15x + 6x^2)]^2$, $x_k = k/b$, $\beta = q_s/b$ and N_{BI} is the BI concentration.

Impurities may also be potentially trapped at the HJ interface, possibly at the step edges; a dislocation generated may enhance the trapping. When such impurities become charged, the scattering from charges located at the interface is described by the relaxation time[22]

$$\tau_{\mathrm{IFC}}^{-1} = C_0 \frac{b^6 N_{\mathrm{IFC}}}{k^2} \int_0^{2k} dq \frac{q^2}{P_o(q,b)(4k^2 - q^2)^{1/2}}. \tag{16}$$

3. Interface roughness scattering

The strength of IFR scattering in a particular sample is determined by the actual morphology of the interfaces. The random fluctuations of a HJ interface from its ideal flat boundary are described by an autocorrelation function.[27] The interface is regarded as consisting of terraces of a few nanometer in size separated by atomic steps of a few tenths of a nanometer and characterized, respectively, by two parameters—correlation length Λ and the rms height Δ. Based on TEM of Si/SiO_2 interfaces it has been demonstrated that the measured roughness data is better described by the exponential correlation function. Due to lack of similar data for GaN/AlGaN interfaces, we assume the roughness of the GaN/AlGaN HJ interface also to be described by the exponential auto covariance function. The relaxation time is given by[19,27]

$$\tau_{\mathrm{IFR}}^{-1} = \frac{m^* \Delta^2 \Lambda^2}{2\hbar^3} \int_0^{2\pi} d\theta (1 - \cos\theta) \frac{\Gamma^2(q)}{\varepsilon^2(q)} (1 + (q^2\Lambda^2/2))^{-3/2}, \tag{17}$$

where $q = 2k \sin(\theta)$ and $\Gamma(q)$ is given by $\Gamma = (4\pi e^2/\kappa_s)(n_{\mathrm{depl}} + n_s/2)$.

4. Acoustic phonon scattering

For the low temperatures of interest, we consider the scattering of the electrons in the GaN channel to arise from bulk acoustic phonons via deformation potential and piezoelectric couplings and assume the contribution from interface phonons to be insignificant. Assuming the scattering to be quasielastic and taking into consideration the degeneracy of the 2DEG, the relaxation time for acoustic phonon scattering can be expressed as[28]

$$\tau_j^{-1} = \frac{m^*}{\hbar^3 \pi^2} \int_0^{\pi} d\theta (1 - \cos\theta) \int_0^{\infty} dq_Z |I(q_Z)|^2 \frac{|C_j(\mathbf{Q})|^2}{\varepsilon^2(q)} \Delta(E) \tag{18}$$

where $\Delta(E) = \{N_Q[1 - f_0(E + \hbar\omega_Q)] + (N_Q + 1)[1 - f_0(E - \hbar\omega_Q)]\}/[1 - f_0(E)]$ and $|I(q_z)|^2 = b^6/(b^2 + q_z^2)^3$. $\cdot\hbar\omega_Q$ is the energy of a phonon with wave vector $\mathbf{Q} \equiv (\mathbf{q}, q_z)$ and N_Q the phonon occupation number. The matrix element $|C_j(\mathbf{Q})|^2$ is given by $|C_{\mathrm{DP}}(\mathbf{Q})|^2 = E_d^2 \hbar Q/2\rho u_l$, for deformation potential (j=DP) scattering and $|C_{\mathrm{PZ},a}(\mathbf{Q})|^2 = \hbar e^2 H_a(Q)/2\rho u_a Q$ for piezoelectric (j=PZ) scattering. The explicit forms of the function $H_a(Q)$ for longitudinal ($\alpha = l$) and transverse ($\alpha = t$) acoustic phonons, in the case of WZ GaN, are given by[29] $H_l(Q) = (h_a^2/48)(15f_0 - 33f_1 + 12f_2 - f_3) + (h_a h_b/4)(3f_0 - 5f_1 + f_2) + (h_b^2/2)(f_0 - f_1)$ and $H_t(Q) = (h_a^2/48)(3f_0 + 3f_1 - 6f_2 + f_3) + (h_a h_b/4)(f_0 + f_1 - f_2) + h_{15}^2 f_0$. Here, the form factors f_n, arising from the anisotropy of the piezoelectric interaction are given by $f_0 = (8 + 9w + 3w^2)/8(1 + w)^3$, $f_1 = 3w(5 + 4w + w^2)/8(1 + w)^4$, $f_2 = 3w^2(8 + 5w + w^2)/4(1 + w)^5$, and $f_3 = 3w^3(35 + 18w + 3w^2)/4(1 + w)^6$, and $h_a = h_{33} - h_b$ and $h_b = h_{13} + 2h_{15}$, h_{ij} being the components of the piezoelectric tensor.

III. RESULTS AND DISCUSSION

We have performed numerical calculations of S_d of a 2DEG at a GaN/AlGaN HJ, using Eqs. (6) and (10)–(18), for parameters characteristic of WZ GaN:[30] $m^* = 0.22\ m_e$, $\rho = 6.1$ gm cm^{-3}, $u_l = 6.56 \times 10^5$ cm s^{-1}, $u_t = 2.68 \times 10^5$ cm s^{-1}, $E_d = 8.3$ eV, $\kappa_s = 9.5$, $h_{33} = 10.86 \times 10^7$ V/cm, $h_{31} = -3.91 \times 10^7$ V/cm, $h_{15} = -3.57 \times 10^7$ V/cm. The other parameters chosen are typically used in the analyses of mobility: $N_{\mathrm{BI}} = 10^{14}$ cm^{-3}, $N_{\mathrm{RI}} = 0.5 \times 10^{17}$ cm^{-3},[4,9] $a_c = -8.0$ eV, $b_e \equiv a_0$ (the lattice constant) = 3.189 Å, $c_0 = 5.185$ Å, $\gamma = 0.3$,[6,14] $\Lambda = 22$ Å, $\Delta = 4$ Å,[6,9,21] $n_{\mathrm{depl}} = 5.0 \times 10^{10}$ cm^{-2},[28] and $N_{\mathrm{IFC}} = 10^{11}$ cm^{-2}.[31] Depending on the growth conditions of the sample, typical dislocation densities, N_{dis}, range from 10^8 cm^{-2} to 10^{10} cm^{-2}.[7,11] In Eq. (10), the filling factor f, whose value depends on the carrier and doping concentrations, ranges from 0 to 1. We take $f = 1$, that is, all the acceptor states in the dislocation are filled. Furthermore, the range of electron concentrations ($n_s = 1 - 5 \times 10^{12}$ cm^{-2}) considered ensures that the Fermi energy $E_F (= \pi\hbar^2\ \mathrm{n_s/m^*})$ lies well below the second electric subband energy.

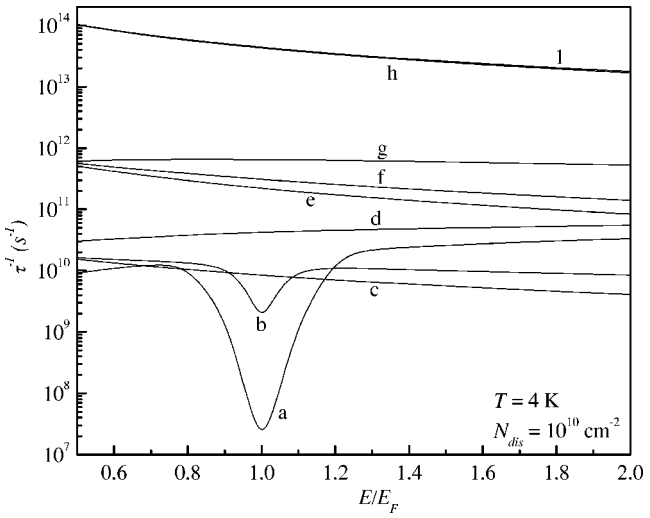

FIG. 1. Energy dependence of electron relaxation rates in GaN/AlGaN HJs at $T = 4$ K with $n_s = 2 \times 10^{12}$ cm^{-2} due to scattering from acoustic phonons via deformation potential (curve a) and piezoelectric (curve b) fields, background impurities (curve c), dislocations via strain field (curve d), interface charges (curve e), remote impurities (curve f), interface roughness (curve g), and dislocations via coulomb field (curve h). Curve 1 denotes the overall contribution.

With a view to better understand the relative importance of the various scattering mechanisms described, in determining the low-temperature S_d, we first examine the variation of their relaxation rates $\tau^{-1}(E)$ as a function of electron energy, E. Figure 1 depicts the energy dependence of the various individual relaxation rates calculated using Eqs. (10), (12), and (14)–(18), for a typical value of $n_s = 2 \times 10^{12}$ cm^{-2} at $T = 4$ K.[32] With increase in E, the scattering rates due to BIs (curve c), IFC (curve e), RIs (curve f), and DC (curve h) decrease contrary to the case of DS (curve d). The rate due to IFR (curve g) at first increases and then decreases with energy, E. In the case of acoustic phonon scatterings, τ_{DP}^{-1} (curve a) and τ_{PZ}^{-1} (curve b), calculated using (18), show an energy dependence similar to that observed in the case of GaAs/AlGaAs HJs;[28] the characteristic dips in the narrow region around E_F arise due to the factor $\Delta(E)$. Since S_d is sensitive to the scattering mechanism, the strong energy dependence of these scattering rates around E_F is expected to influence the behavior of S_d in the BG regime.

For the degenerate 2DEG at the GaN/AlGaN HJ, the overall relaxation rate τ^{-1} may be calculated using Mattheissen's rule

$$\tau^{-1} = \tau_{\mathrm{DP}}^{-1} + \tau_{\mathrm{PZ}}^{-1} + \tau_{\mathrm{BI}}^{-1} + \tau_{\mathrm{RI}}^{-1} + \tau_{\mathrm{IFC}}^{-1} + \tau_{\mathrm{IFR}}^{-1} + \tau_{\mathrm{DC}}^{-1} + \tau_{\mathrm{DS}}^{-1}. \tag{19}$$

Curve 1 in Fig. 1 shows the energy dependence of the overall relaxation rate, τ^{-1}. It is found that the dominant contributions to τ^{-1} arise from charged dislocation and interface

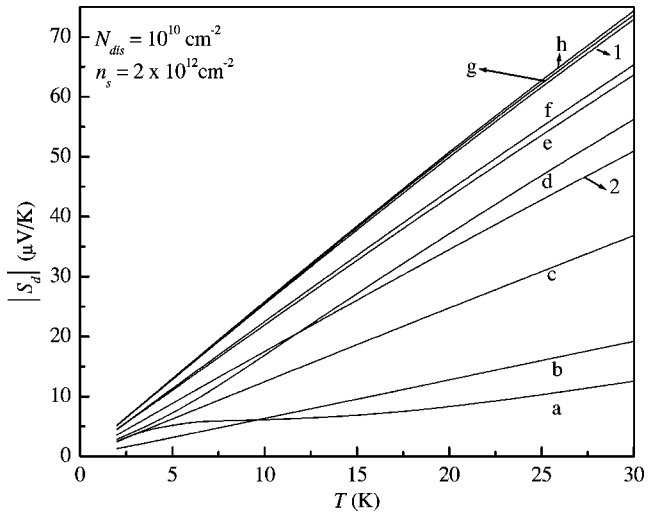

FIG. 2. Variation of S_d with temperature in GaN/AlGaN HJs with $n_s=2\times10^{12}$ cm^{-2}. Curves a–h represent individual contributions to S_d from acoustic phonons via deformation potential, dislocations via strain field, interface roughness, acoustic phonons via piezoelectric fields, background impurities, remote impurities, dislocations via coulomb field, and interface charges, respectively. Curve 1 denotes the total contribution. Curve 2 depicts the variation neglecting contribution from dislocations.

roughness scatterings. This is consistent with the recent observations of Syed *et al.*[32] Also, the factor $[1-\cos(\theta)]$ in the integrand for the relaxation rates indicates that it is the large-angle scatterers that contribute significantly.[20,28] For the values of the parameters employed, the contributions to τ^{-1} from IFC and RIs are found to be about two orders of magnitude small; the contribution from BIs is about four orders of magnitude small. In the case of acoustic phonons, the contributions at $E=E_F$ from DP and PZ scatterings are, respectively, nearly six and four orders of magnitude small, with the contribution from τ_{PZ}^{-1} being larger. With decrease in temperature the dips become deeper.

Figure 2 depicts the temperature variation of S_d, calculated using Eq. (6). Curves a–h show the variation of the individual contributions to S_d, for $n_s=2\times10^{12}$ cm^{-2}, when the electrons are scattered by DP phonons, DS, IFR, PZ phonons, BIs, RIs, DC, and IFC, respectively. Curve 1 represents the variation of the total contribution to S_d, calculated with an overall relaxation time given by Eq. (19). It is seen that S_d, for the various mechanisms (except for acoustic phonon scattering), increases almost linearly with T, as expected [Eq. (8)] for a degenerate 2DEG. The behavior of S_d, it is clear from Eq. (6), depends on the relaxation rates and their energy dependence. Thus, although a scattering mechanism may have a high relaxation rate its contribution to S_d may be small because of its less dependence on energy. For the range of temperatures considered and for the values of parameters chosen, S_d (curve 1) is found to be dominated by charged dislocations. For $N_{\mathrm{dis}}<10^7$ cm^{-2}, S_d is dominated by interface scattering (IFR and IFC). Although PZ phonons influence S_d more than the DP phonons, the total contribution from acoustic phonons is found to be only about 2% of the total S_d even at 30 K. However, it may be noted that, both the contributions do not depend linearly on T. The departure from the linear behavior is clearly seen in the case of DP scattering in the temperature range $5<T<20$ K. Such behavior stems from the energy dependence of the relaxation rates $\tau_{\mathrm{DP}}^{-1}(E)$ and $\tau_{\mathrm{PZ}}^{-1}(E)$ around E_F. Curve 2 in Fig. 2 shows the temperature dependence of S_d neglecting the contribution from dislocations. We note that, in the absence of dislocation scattering, scatterings at the interface, namely, IFR and IFC, become important; RIs also contribute. Calculations, by the present authors, of S_d in AlGaN/GaN/AlGaN quantum wells of both ZB and WZ structures have shown that, in the absence of dislocations, S_d is determined at low temperatures by remote impurities, interface roughness and piezoelectric phonons.[33]

It may be observed that, for the temperature range of interest ($T<30$ K) and typical carrier densities ($n_s=2\times10^{12}$ cm^{-2}) considered, the thermal energy k_BT is much smaller than the Fermi energy and only a small fraction of acoustic phonons having wavevector $q\leqslant2k_F$ can interact with the degenerate 2DEG. The transition into the Bloch-Grunessein (BG) regime, where acoustic phonon energies are comparable to k_BT and phonons with $q\sim2k_F$ cease to be thermally excited, roughly occurs at a temperature $T_{\mathrm{BG}}\sim2k_F\hbar u_\alpha/k_B$. For longitudinal and transverse acoustic modes the values of T_{BG} are 35.5 K and 14.9 K, respectively. The BG transition is a consequence of the factor $\Delta(E)$ [in Eq. (18)], which strongly reduces the acoustic phonon relaxation rates,[28,30] as in Fig. 1. In this context it may be noted that, Stormer *et al.*[34] have observed rapid decrease (increase) in the acoustic-phonon-limited scattering rate (mobility) of 2DEG in ultra pure GaAs/AlGaAs heterostructures at low temperatures. In view of the strong energy dependence of scattering rates around E_F, both in the case of GaN (curves a and b in Fig. 1) and GaAs[28] systems, and thermopower being sensitive to the scattering mechanisms, it should be possible to observe the transition into BG regime in the acoustic-phonon-limited thermopower.[35]

Figure 3 shows the dependence of S_d, on dislocation densities. Curves a, b, and c represent the temperature variation of S_d for $N_{\mathrm{dis}}=10^8$, 10^9, and 10^{10} cm^{-2}, respectively with $f=1$. Since, in Eq. (10), ρ_L and N_{dis} appear as a product, Fig. 3 may be also be used to understand the dependence of S_d on the dislocation charge density. It may be noted that, with increase of dislocation density the magnitude of S_d increases, though not proportionally.

Figure 4 shows the variation of S_d as a function of the electron concentration, n_s, at $T=4$ K. Curves a–g show the variation of the individual contributions to S_d from DS, IFR, DP+PZ, BI, RI, DC, and IFC scatterings, respectively. Curve 1 represents the total contribution to S_d. For the temperatures and the range of concentrations considered, we find that S_d decreases with increase in n_s, at first rapidly and then slowly. S_d is found to be dominated by DC for lower values of n_s, and by IFR for higher values. A similar behavior is observed in the case of carrier mobilities.[6,10,12] This is consistent with the observation that as n_s increases the distribution of the electrons in the well changes becoming more confined to the GaN/AlGaN interface. The influence of dislocation scattering from the strain fields is found to be negligible compared to that from the Coulomb field. It is also found that, the

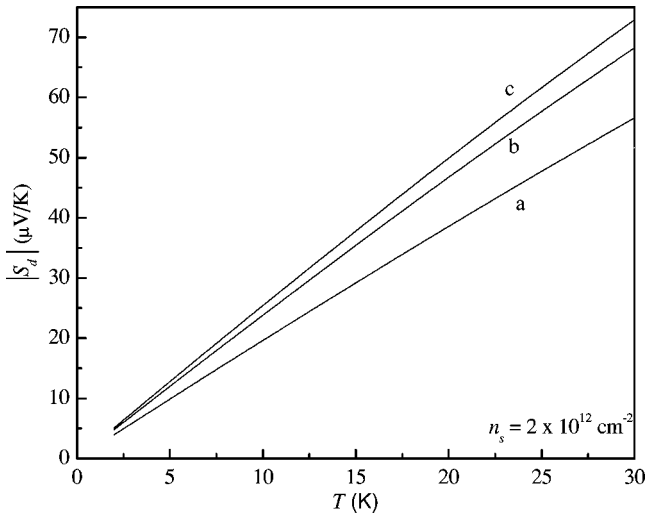

FIG. 3. Temperature variation of S_d in GaN/AlGaN HJs with $n_s=2\times10^{12}$ cm^{-2} for three values of $N_{\rm dis}$: 10^8 cm^{-2} (curve a), 10^9 cm^{-2} (curve b), and 10^{10} cm^{-2} (curve c).

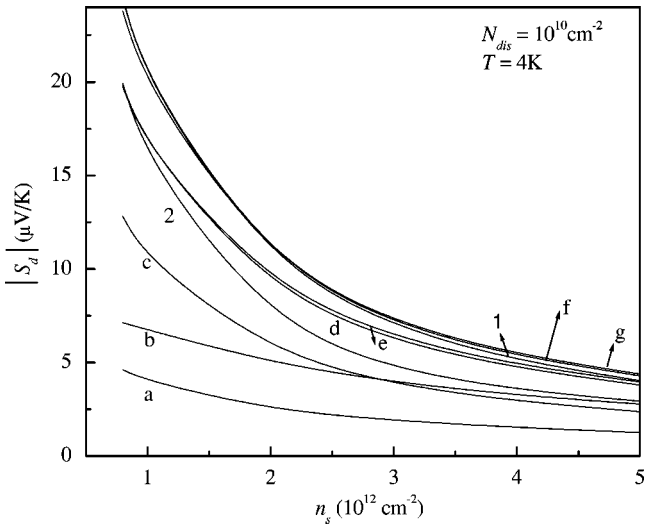

FIG. 4. Variation of S_d with n_s for GaN/AlGaN HJs at $T=4$ K. Curves a–g represent individual contributions to S_d from dislocations via strain field, interface roughness, acoustic phonons via deformation potential and piezoelectric fields, background impurities, remote impurities, dislocations via coulomb field, and interface charges, respectively. Curve 1 denotes the total contribution. Curve 2 depicts the variation neglecting contribution from dislocations.

contribution to S_d from impurity scattering becomes appreciable at lower electron concentrations. Curve 2 in Fig. 4 shows the carrier concentration dependence of S_d for samples devoid of dislocations. S_d is found to be influenced by RI and IFC scatterings for $n_s<2\times10^{12}$ cm^{-2} and is controlled by IFR scattering for $n_s>3\times10^{12}$ cm^{-2}.

From Figs. 2 and 4 it is clear that the contributions from DS and IFR are smaller than those from RI, BI, IFC, and DC. This can also be seen from the values of the energy-dependence exponent p of Eq. (9) for individual scattering mechanisms. We have calculated the values of p for $n_s=2\times10^{12}$ cm^{-2}, and find it to be nearly −0.5 for DS, 0.1 for IFR, 1.0 for RI, 1.0 for BI, 1.3 for IFC, and 1.3 for DC. The value of p for the overall scattering rate is found to be 1.28, with and without IFC contribution, implying that charged dislocation scattering is the dominant mechanism. Dislocation scattering, thus, plays an important role in determining the low-temperature S_d. The effect of dislocations is to alter S_d, the effect being more for lower values of n_s. It may be observed that the contributions to S_d from remote and background impurities are also significant.

IV. CONCLUSION

In conclusion, we have presented detailed calculations of low-temperature S_d of a 2DEG realized at a GaN/AlGaN HJ assuming the electrons to be scattered by various scattering mechanisms operative in the system. We find that the contribution due to charged dislocations is important in determining the diffusion thermopower. With attempts being made[3] at reducing the threading-dislocation densities using novel growth techniques, it would be interesting to observe, in pure samples, without dislocations at lower temperatures, a signature of the onset of the BG regime in thermopower studies[35] similar to that observed in mobilities of such systems. At an interface, although surface acoustic phonons can as well be excited, in the present work bulk phonons are assumed to provide a qualitatively correct description of the electron-phonon interaction.[36] The influence of surface/confined acoustic phonons on thermopower in general, in 2DEG systems is being pursued. Experimental studies of TEP will test the predictions presented in this work.

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[1] O. Ambacher, J. Phys. D **31**, 2653 (1998).
[2] H. Morkoc, *Nitride Semiconductors and Devices* (Springer-Verlag, Berlin, 1999).
[3] T. Miyajima, T. Tsuyoshi, T. Asano, K. Yanashima, S. Kijima, T. Hino, M. Takeya, S. Uchida, S. Tomiya, K. Funato, T. Asatsuma, T. Kobayashi, and M. Ikeda, J. Phys.: Condens. Matter **13**, 7099 (2001).
[4] L. Hsu and W. Walukiewicz, Phys. Rev. B **56**, 1520 (1997).
[5] B. K. Ridley, B. E. Foutz, and L. F. Eastman, Phys. Rev. B **61**, 16 862 (2000).
[6] R. P. Joshi, S. Viswanadha, B. Jogai, P. Shah, and R. D. del Rosario, J. Appl. Phys. **93**, 10 046 (2003).
[7] D. C. Look and J. R. Sizelove, Phys. Rev. Lett. **82**, 1237 (1999).
[8] C. Mavroidis, J. J. Harris, M. J. Kappers, and C. J. Humphreys, J. Appl. Phys. **93**, 9095 (2003).
[9] S. Gokden, Physica E (Amsterdam) **23**, 19 (2004).

[10] D. Zanato, S. Gokden, N. Balkan, B. K. Ridley, and W. J. Schaff, Semicond. Sci. Technol. **19**, 427 (2004).
[11] N. G. Weimann, L. F. Eastman, D. Doppalapudi, H. M. Ng, and T. D. Moustakas, J. Appl. Phys. **83**, 3656 (1998).
[12] D. Jena and U. K. Mishra, Appl. Phys. Lett. **76**, 1707 (2000).
[13] H. M. Ng, D. Doppalapudi, T. D. Moustakas, N. G. Weimann, and L. F. Eastman, Appl. Phys. Lett. **73**, 821 (1998).
[14] D. Jena, A. C. Gossard, and U. K. Mishra, Appl. Phys. Lett. **80**, 64 (2002).
[15] F. A. Ponce, MRS Bull. **22**, 51 (1997).
[16] F. J. Blatt, P. A. Schroeder, C. L. Foiles, and D. Greig, *Thermoelectric Power of Metals* (Plenum Press, New York, 1976).
[17] B. L. Gallagher and P. N. Butcher, in *Handbook on Semiconductors*, edited by P. T. Landsberg (Elsevier, Amsterdam, 1992) Vol. 1 p. 817.
[18] R. Fletcher, Semicond. Sci. Technol. **14**, R1 (1999).
[19] T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
[20] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders College Publishing, New York, 1976).
[21] V. C. Karavolas and P. N. Butcher, J. Phys.: Condens. Matter **3**, 2597 (1991).
[22] W. Walukiewicz, H. E. Ruda, J. Lagowski and H. C. Gatos, Phys. Rev. B **30**, 4571 (1984).
[23] C. Shi, P. M. Asbeck, and Edward T. Yu, Appl. Phys. Lett. **74**, 573 (1999).
[24] J.-L. Farvacque, Phys. Rev. B **62**, 2536 (2000).
[25] P. J. van Hall, T. Klavar, and J. H. Wolter, Semicond. Sci. Technol. **3**, 120 (1988).
[26] B. K. Ridley, Semicond. Sci. Technol. **11**, 1339 (1996).
[27] B. K. Ferry and S. M. Goodnick, *Transport in Nanostructures* (Cambridge University Press, Cambridge, 1997).
[28] T. Kawamura and S. Das Sarma, Phys. Rev. B **45**, 3612 (1992).
[29] P. Tripathy and B. K. Ridley, Phys. Rev. B **66**, 195301 (2002).
[30] N. A. Zakhleniuk, C. R. Bennett, M. Babiker, and B. K. Ridley, Appl. Phys. Lett. **75**, 1565 (1999).
[31] C. J. Emeleus, T. E. Whall, D. W. Smith, R. A. Kublak, E. H. C. Parkar, and M. J. Kearney, J. Appl. Phys. **73**, 3852 (1993).
[32] S. Syed, M. J. Manfra, Y. J. Wang, R. J. Molnar, and H. L. Stormer, Appl. Phys. Lett. **84**, 1507 (2004).
[33] M. D. Kamatagi, N. S. Sankeshwar, and B. G. Mulimani, *Proc. Solid State Phys. Symp.*, Vol. 46C, (2003).
[34] H. L. Stormer, L. N. Pfeiffer, K. W. Baldwin, and K. W. West, Phys. Rev. B **41**, 1278 (1990).
[35] N. S. Sankeshwar, M. D. Kamatagi, and B. G. Mulimani (unpublished).
[36] A. Knabchen, cond-mat/9702150 (unpublished).