Analysis of the temperature dependent thermal conductivity of silicon carbide for high temperature applications

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The temperature dependent thermal conductivity of silicon carbide has been calculated taking into account the various phonon scattering mechanisms. The results compared very well with available experimental data. The inclusion of four-phonon processes is shown to be necessary for obtaining a good match. Several important phonon scattering parameters have been extracted in this study. Dislocations are shown to have a strong effect at 300 K, but not as much at the higher temperatures.
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INTRODUCTION

Silicon carbide (SiC) based electronic devices and circuits are presently being developed for use in high-temperature, high-power, and/or high-radiation conditions under which conventional semiconductors cannot perform adequately.[1–5] The projected advantages of SiC are associated with its inherent material properties. These include exceptionally high breakdown fields, a large band gap, high electron saturation drift velocities, and large thermal conductivity values. This makes SiC an attractive candidate for devices requiring low leakage currents, high cut-off frequencies at large voltages, in high-temperature electronics, and for high-power microwave operation. Theoretical predictions suggest that SiC power metal–oxide–semiconductor field effect transistors, thyristors, and diode rectifiers would offer significant advantages over their silicon and GaAs counterparts in high-frequency, high-power circuits, and yet require die sizes nearly 20 times smaller.[6]

Despite promising trends, superior quality SiC high-power devices are not being realized presently. While small-area, low-current, low-voltage power SiC devices have successfully been developed, there has been limited progress in the large-area, high-current, high-voltage (i.e., operation near the breakdown field) arena. The presence of a high density of crystallographic defects in commercial SiC wafers (with surfaces perpendicular to the *c* axis), continues to hamper development. Of the various defects, micropipes (i.e., hollow-core screw dislocations) have been the most studied,[7–9] and are known to cause premature breakdown point failures at electric fields well below the breakdown threshold. However, with improvements in processing technology, micropipe defect densities have steadily been reduced and are now below $1/cm^2$ in the best prototype wafers.[10] The focus will, therefore, naturally begin to shift towards other defects such as elementary, closed-core dislocations. Closed-core screw dislocations are present in all commercial SiC wafers and homoepitaxial layers that are the starting material for SiC electronic devices, due to their nonterminating nature. Densities on the order of thousands/cm^2 have been reported,[11,12] and experimental studies of dislocation effects on the electrical behavior are only beginning to emerge. For example, it has recently been demonstrated that screw dislocations can degrade the reverse leakage and breakdown properties of 4H-SiC p^+n diodes[13] and lead to local decreases in carrier lifetimes.[14] In experiments, diodes containing dislocations were shown to exhibit higher pre-breakdown reverse currents, displayed softer breakdown thresholds, and led to the formation of highly localized filamentary microchannels. In light of the above, it becomes important to analyze the impact of dislocations on the response characteristics of SiC devices containing such defects. In a previous study,[15] some of the possible physics behind the electrical behavior were examined. Trapped charge modeled at the dislocation induced defect sites was shown to alter the internal electric field distribution. This, in turn, could affect the ionization rates due to their strongly nonlinear field dependence, and lead to current increases of the SiC diode under reverse bias conditions.

Here, we examine thermal effects in SiC material and the possible role of dislocations on the internal temperature of SiC devices. The thermal issue is especially important for SiC as this material is a primary candidate for high-temperature, high-voltage applications. The electrothermal aspects are also critical in determining the operating limits and boundaries for safe device operation. The thermal conductivity parameter, *k*, depends on an effective phonon relaxation time ϑ_{pr} which is shaped by the combined effects of the various phonon processes.[16,17] These typically include normal three-phonon processes,[18,19] boundary scattering,[20,21]

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isotope/point defect interactions,[22] and the umklapp mechanism.[23,24] If the operating temperatures are not very low, boundary scattering is relatively negligible and the value of k begins to decrease monotonically with temperature due to increases in the combined phonon scattering rate. For bulk SiC, this regime of decreasing thermal conductivity would be encountered for operation at temperatures of 300 K and beyond. Recent experimental studies on 6H-SiC confirm this monotonically decreasing trend in thermal conductivity,[25–27] and reveal an approximate T^{-n} functional form, with $1<n<2$. With such thermal conductivity reductions, device self-heating under high-voltage operation is expected to have a strong influence. Consequences include performance degradation and adverse affects on device stability. It might be mentioned in this regard that there are already reports of filamentary conduction[13] and device failure in SiC at high bias.[28] Although the precise cause remains unclear, internal temperature increases appear to be involved.

Apart from the effects on carrier mobilities and device stability, the device operating temperatures have recently been shown to influence impact ionization rates. Higher ionization coefficients were observed in SiC material containing dislocations and defects, and their values increased with temperature.[29] This trend is contrary to that generally seen in silicon and predicted for pure semiconductor materials.[30] With increasing temperature, the inelastic phonon scattering increases, making it less likely for a ''lucky electron or hole'' to remain within the high-energy distribution and subsequently undergo an impact ionizing collision. The ionization rates are thus expected to reduce with increasing temperature. The phenomenon in SiC is not well understood, but is thought to be linked to dislocation physics.[29,31] We believe charge trapping followed by field- and temperature-assisted detrapping in SiC containing dislocations is a likely cause.[15] In any case, given the temperature sensitivity, it is important to evaluate and characterize the device operating temperatures. Last but not least, the presence of additional phonon scattering at the defects and dislocations in SiC is expected to reduce heat transport, making the thermal issue even more critical. As first pointed out by Klemens,[32] the strain fields of screw and edge dislocations contribute to such additional phonon scattering. This can lead to reductions in thermal conductivity, as has been observed experimentally in SiC (Ref. 33) and other materials.[34]

In light of the above, a thermal analysis for SiC devices becomes relevant and germane. In this article, the temperature dependence of SiC thermal conductivity has been probed taking into account the various phonon scattering mechanisms. The results are carefully compared with available experimental data, and found to be in very good agreement. In the process of such a comparison, several important parameters associated with the various phonon processes have been extracted in this study. Finally, the role of dislocation scattering and associated thermal conductivity reductions is also discussed.

SIMULATION DETAILS

We begin by focusing on the thermal conductivity parameter, $k(T)$, and providing some relevant comments with regard to its expected temperature dependence and the role of various constituent phonon scattering processes. As already mentioned, recent experimental data on 6H-SiC has yielded the following temperature dependent expression:[26] $k(T)=4.517\times10^{5}\,T^{-1.29}\,\mathrm{W\,m^{-1}\,K^{-1}}$. This temperature dependence is dictated by the collective contribution of several phonon scattering mechanisms. To the best of our knowledge, the relative role of the constituent scattering processes has not been analyzed, nor have the parameters associated with the interactions been extracted for SiC. Furthermore, the measurements were made on actual samples, which might or might not have been relatively defect free. This point has not been explicitly stated or clarified in Ref. 26, so it needs to be examined. The presence of a high-density network of basal plane dislocations, often reported in SiC wafers, could reduce thermal conductivity. Here, we have carried out a theoretical analysis to probe some of the thermal conductivity issues based on the theory developed by Callaway[16] and by Slack and co-workers.[24] The following assumptions have implicitly been made. (1) Phonons transport all of the heat. Hence, electronic contributions or radiation transport are neglected. Justification is partially based on a recent study that confirms the weakness of these processes in SiC.[26] (2) The phonons can be represented by a Debye-type approximation with a single frequency-independent phonon velocity, and a maximum frequency fixed by the Debye temperature. Although the presence of defects produces variations in the atomic mass and force constants, thereby changing the phonon spectra, this effect has been neglected here. (3) Anisotropic effects have also been ignored. (4) The relaxation time approximation has been used for simplicity since expressions for the individual relaxation processes are well known. (5) It has been assumed that contributions from the normal processes (i.e., momentum conserving) can be ignored in the temperature range of 300–800 K that is of interest for the present calculations. This range was chosen so as to remain below the 1200 K Debye temperature for SiC.

Basically, the thermal conductivity can be expressed in terms of the effective phonon relaxation time ϑ_{pr} and is given as[16]

$$k(T)=(4\pi k_B/v_s)(k_BT/h)^3 \times\int_0^{\theta/T} x^4\vartheta_{pr}(x)[e^x/(e^x-1)^2]dx, \tag{1}$$

where θ is the Debye temperature, v_s the average velocity of sound, h is Planck's constant, k_B the Boltzmann constant, and $x=(h\omega)/(2\pi k_BT)$. The phonon time ϑ_{pr} in the above equation can roughly be obtained based on the relaxation time approximation (RTA). In the RTA, each phonon scattering mechanism is treated as making a separate and independent contribution to the overall relaxation rate ϑ_{pr}^{-1}. Thus, in terms of the ith scattering mechanism, the following equation results:

$$\vartheta_{pr}^{-1}=\sum_i \vartheta_i^{-1}=\vartheta_I^{-1}+\vartheta_U^{-1}+\vartheta_D^{-1}+\vartheta_B^{-1}+\vartheta_N^{-1}+\vartheta_{4P}^{-1}, \tag{2}$$

where ϑ_I, ϑ_U, ϑ_D, ϑ_B, ϑ_N, and ϑ_{4P} are the relaxation times associated with isotope scattering, the Umklapp process, dislocation scattering, the phonon–boundary interactions, normal phonon processes, and four-phonon events, respectively. Of these, the normal processes do not significantly affect the thermal conductivity much since the phonon momentum is conserved. Hence, their contribution has been neglected in this treatment. The four-phonon processes, as suggested by Pomerranchuk,[35] play a role at high temperatures, and have been considered here. As the results will show, the four-phonon process appears to be fairly important in SiC, and good agreement with experimental data cannot be obtained without its inclusion. Applying the well known expressions to the processes[16,22] leads to the following mathematical expressions for the scattering rates: $\vartheta_I^{-1}=A\omega^4$, $\vartheta_U^{-1}=BT\exp[-\theta/(aT)]\omega^2$, $\vartheta_B^{-1}=v_s/L$, $\vartheta_D^{-1}=DN_Db^2\omega$, and $\vartheta_{4P}^{-1}=CT^2\omega^2$, where A, B, C, and D are material constants. The parameter ''a'' for the Umklapp process is adjustable. Previous reports on several semiconductor materials suggest that the $1\leqslant a\leqslant 3$ range yields a good fit to experimental data.[24] For SiC, a value of $a=1$ has been used recently by Muller *et al.*[26] As pointed out by Klemens,[22] if a number of parallel dislocations are grouped together in a region whose spatial extent is small compared to the phonon wavelength, their scattering can be reinforced. The overall effect can then be treated as a single dislocation having a Burgers vector given by the sum of individual dislocations. Numerically, this can be folded into the D parameter given above. The overall effective phonon relaxation time thus has the following general form:

$$\vartheta_I^{-1}=A\omega^4+BT\exp[-\theta/(aT)]\omega^2+CT^2\omega^2+DN_Db^2\omega+v_s/L, \tag{3}$$

where L is the characteristic length scale of the sample, ω the phonon frequency, N_D the dislocation density per unit area, and b the magnitude of the Burgers vector. Using Eq. (3) in Eq. (1) then leads to the following conductivity expression:

$$k(T)=[4\pi k_B/v_s](k_BT/h)^3\int_0^{\theta/T}\{x^4/[P_1x^4+(P_2+P_3)x^2+P_4x+v_s/L]\}[e^x/(e^x-1)^2]dx, \tag{4}$$

where $P_1=A(2\pi k_BT/h)^4$, $P_2=BT^3\exp[-\theta/(aT)]\times(2\pi k_B/h)^2$, $P_3=CT^2(2\pi k_BT/h)^2$, and $P_4=DN_Db^2\times(2\pi k_BT/h)$. It is perhaps instructive to examine the expected behavior of $k(T)$ at high temperatures. At 300 K and beyond, the $x^2[e^x/(e^x-1)^2]$ term approaches unity. Also, as is well known, the boundary scattering becomes negligibly small. Equation (4) then yields

$$k(T)=[4\theta k_B/v_s](k_BT/h)^3\times\int_0^{\theta/T}\{x^2/[P_1x^4+(P_2+P_3)x^2+P_4x]\}dx. \tag{5}$$

In the absence of dislocation scattering, the above equation works out to

$$k(T)\sim T^{-0.5}\{C_1\exp[-\theta/(aT)]+C_2T\}^{-0.5}\times\tan^{-1}(\theta/\{C_1T\exp[-\theta/(aT)]+C_2T^2\}^{0.5})\sim T^{-0.5}\{C_1\exp[-\theta/(aT)]+C_2T\}^{-0.5}, \tag{6}$$

where C_1 and C_2 are temperature independent constants and arise from factors P_2 and P_3. Neglecting the C_1 factor leads roughly to a $k(T)\sim T^{-1}$ dependence. However, the actual variation is more complicated since the C_1 factor cannot really be neglected since the umklapp processes are quite important. The umklapp process dominance is demonstrated and discussed through numerical computations next. A larger negative exponent value is predicted for the temperature dependence based on Eq. (6) above. Recent experimental reports of the SiC thermal conductivity suggest a $T^{-1.29}$ temperature variation.[26] Since this is close to the approximate analysis discussed above, it is reasonable to conclude that dislocation scattering in the experimental samples was either weak or absent. A numerical analysis that will be presented next shows that good agreement with the experimental data can be achieved without any considerations of the dislocation scattering mechanism. As a final point, data are currently not available for the 4H-SiC polytype. However, one could use Eq. (4) to go from the 6H-SiC to the 4H-SiC parameters. Very roughly, the values would be related to the inverse ratio of the acoustic velocities. Since $v_s|_{4H}\sim v_s|_{6H}=1.3\times10^4\,\mathrm{m\,s^{-1}}$, the same $k(T)=4.517\times10^5\,T^{-1.29}\,\mathrm{W\,m^{-1}\,K^{-1}}$ expression can roughly be used for the 4H-SiC thermal conductivity as well.

TABLE I. Parameters used for thermal conductivity calculations for SiC.

Parameter	Value
Debye temperature (K)	1.2×10^3
Acoustic velocity ($\mathrm{m\,s^{-1}}$)	1.3×10^4
Boundary scattering length L (m)	0.5×10^{-2}
Isotope scattering parameter A ($\mathrm{s^3}$)	8.46×10^{-45}
Umklapp parameter B ($\mathrm{s\,K^{-1}}$)	6.1626×10^{-20}
Parameter b for umklapp process	1.0
Four-phonon process parameter C ($\mathrm{s\,K^{-2}}$)	6.9×10^{-23}
Burgers vector b (m)	14.5×10^{-10}

RESULTS AND DISCUSSION

Numerical calculations for the thermal conductivity were carried out based on Eq. (4). Since not all of the scattering parameters are well known for SiC, the intent was to obtain reasonable fitting values for all the parameters through direct comparisons between theory and the available experimental data. In the process, the role of constituent phonon scattering mechanisms was brought out very clearly. Only some of the parameter values for the phonon scattering times are known from the literature.[36,37] Others had to be adjusted in order to achieve a good fit with the experimental data. The overall set of parameters that emerged and were used here are given in Table I. Dislocation scattering was deliberately ignored to begin with. The intent was to ascertain whether it would be possible to achieve a reasonable match with the available

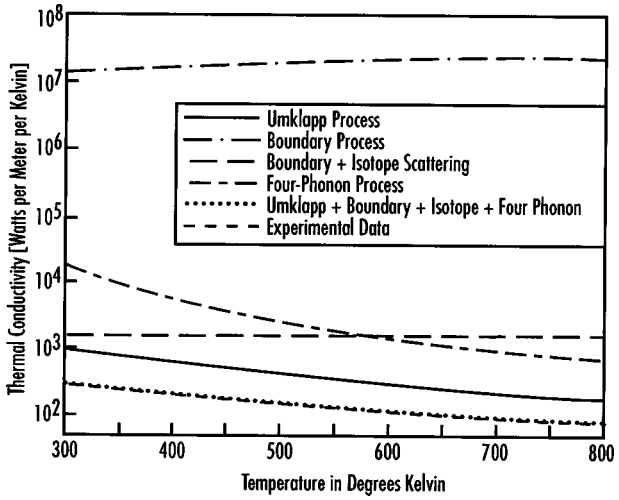

FIG. 1. Simulation results of the temperature-dependent SiC thermal conductivity resulting from a variety of phonon scattering mechanisms. An experimental curve (after Ref. 26) is also shown.

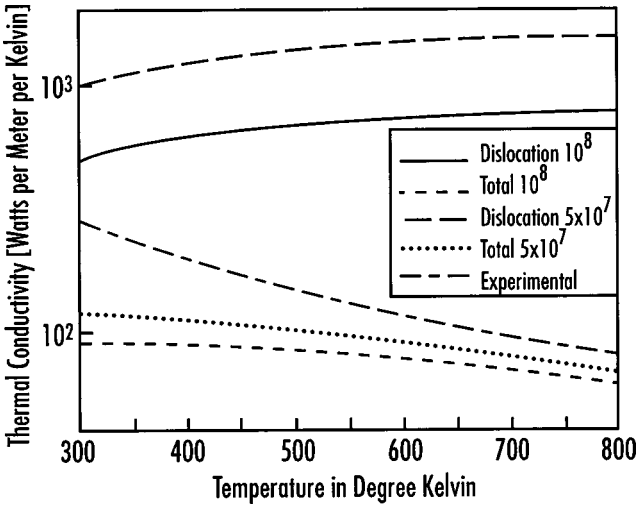

FIG. 3. Predictions of the temperature-dependent thermal conductivity using two values of the dislocation parameter *R*. Experimental data are also shown.

experimental data without the dislocation scattering mechanism. Good agreement would either indicate an absence of dislocations in the experimental samples, or a relatively weak contribution from this scattering process. Figure 1 shows the calculated SiC thermal conductivity associated with the various constituent phonon scattering mechanisms. Experimental data are also given for the 300–800 K range. The comprehensive result reveals a rather good match with the available SiC data. The umklapp process is evidently the strongest in this entire temperature regime. The isotope/defect mechanism is the next most dominant process near room temperature, but is overtaken by four-phonon scattering beyond 600 K. The role of four-phonon scattering, which has been ignored in many previous studies, is brought out more clearly in Fig. 2. Without the four-phonon process, the thermal conductivity resulting from all of the remaining mechanisms is predicted to be much larger than the measured data. In addition, the slope is substantially incorrect in the absence of the four-phonon processes, especially at the lower temperatures. Close agreement between theoretical predictions and the data curve underscores the weakness of dislocation scattering. The role of dislocation scattering is not negated though, since the result might simply have been the consequence of using relatively pure samples in the actual experiments of Muller *et al.*[26]

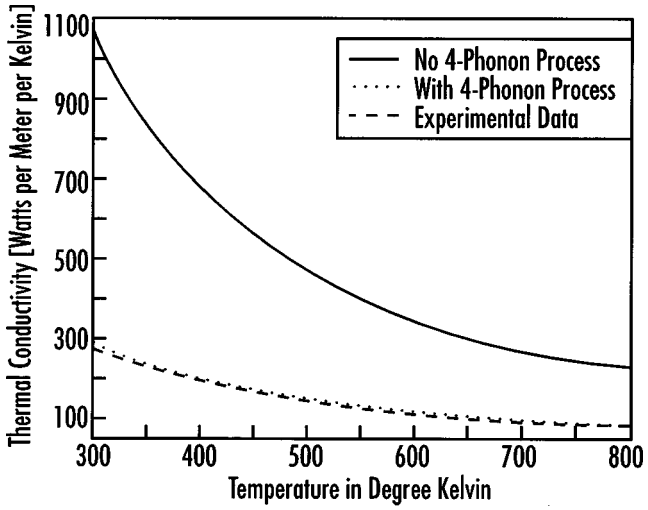

FIG. 2. Simulation predictions of the temperature-dependent SiC thermal conductivity with and without the four-phonon processes being taken into account. Experimental data are shown for comparison.

In order to roughly assess the effect of dislocations on thermal conductivity, the preceding calculations were repeated but with inclusion of the dislocation scattering term. Parameter values for the remaining processes were kept fixed as given in Table I. The P_4 term of Eq. (4) was treated as a variable. Thus denoting $P_4=[DN_Db^2(2Bk_B/h)]T\equiv RT$, the temperature-dependent SiC thermal conductivity was obtained for two values of the parameter *R*. The corresponding curves are shown in Fig. 3 for two values of *R*: $R=5\times10^7$ and $10^8\,\mathrm{s^{-1}K^{-1}}$. The thermal conductivity in Fig. 3 due to the dislocations alone exhibits a monotonic increase with temperature. This trend is opposite that exhibited by all the remaining processes, and demonstrates that dislocation scattering is expected to have an impact primarily at the lower operating temperatures. The total thermal conductivity, taking into account all of the remaining phonon processes, has a value lower than the experimental baseline result, and exhibits a reduced temperature variation. Thermal conductivities as low as 95 $\mathrm{W\,m^{-1}K^{-1}}$ are predicted in Fig. 3 for room temperature operation. The technological implications are obvious. Dislocations lead to the formation of defect states due to internal lattice strain. Charge trapping at these sites can then give rise to *S*-shaped negative differential conductance characteristics[38] and trigger devices into a filamentary mode. High current densities in such filaments, coupled with the strong conductivity decreases with temperature as predicted here, could lead to catastrophic and irreversible failures in SiC devices.

CONCLUSIONS

The temperature dependence of SiC thermal conductivity has been probed in this study taking account of the vari-

ous phonon scattering mechanisms. The process of phonon scattering at screw dislocations due to the internal lattice strain has been included. Such calculations have not been performed previously to the best of our knowledge. It has been demonstrated that the dislocations are likely to affect the thermal conductivity adversely at the lower temperatures. The simulation results were carefully compared with available experimental data, and found to be in very good agreement. The inclusion of four-phonon processes was shown to be necessary for obtaining a good match. In the process of such a comparison, several important parameters associated with the various phonon processes have been extracted in this study.

The role of dislocation scattering was shown to be quite strong at the room temperature value. The implications for technological development of SiC devices are obvious. Structures having screw dislocations should be avoided not only because they reduce the thermal conductivity, but also because they can initiate filamentary conduction, leading to large localized temperature increases.

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