Modeling of the Thermal Conductivity of Polycrystalline GaN Films

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ABSTRACT

We present preliminary results of a theoretical investigation of the thermal conductivity of polycrystalline GaN films. It is assumed that grain boundaries play a major role in limiting the thermal conductivity, which is calculated using the phonon-hopping transport approach. The effect of the grain size, size dispersion, and inter-grain interface structure on the thermal conductivity values is analyzed. The obtained results are compared with available experimental data for polycrystalline films and model predictions for crystalline GaN films.

I. INTRODUCTION

Gallium nitride (GaN) is a wide-bandgap semiconductor, which is well suited for applications in high-power electronic and optoelectronic devices. Due to the high-power density involved, the thermal budget constrains is a very important consideration in designing GaN-based devices. The estimates of temperature rise, and corresponding degradation of the device performance, depend crucially on the values of the thermal conductivity used. The modeling of temperature rise is complicated by the discrepancy of the reported experimental values of the thermal conductivity and its apparent strong dependence on the material quality and concentration of impurities [1].

We have recently calculated the thermal conductivity in wurtzite GaN crystalline films as the function of temperature and density of dislocation lines, dopants and impurities [1-2]. The calculation was based on Klemens’ formulas for the phonon scattering rates [3] and explicitly included three-types of dislocation lines and four impurities typical for GaN. The functional dependence of the thermal conductivity on doping density and temperature in crystalline GaN compared favorably with experimental data quoted in the Ref. [1-2].

In this paper we investigate the thermal conductivity of polycrystalline GaN films, which currently attract significant attention. It is known that the temperature dependence of the thermal conductivity of polycrystalline films is very different from that of crystalline materials. Moreover GaN samples with very large concentration of defects can be considered as disordered material rather than crystal. This requires a different theoretical approach for calculating the thermal conductivity.

In this work we adopt a general formalism for the thermal conductivity in polycrystalline materials proposed by Braginsky et al. [4], apply it to GaN films, and compare the results with experimental data for polycrystalline GaN reported by Daly et al. [5]. The results are then analyzed in order to extract the thermal conductivity

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dependence on the grain size and determine the typical values of inter-grain transparency parameter for acoustic phonons.

II. THEORETICAL MODEL

The thermal conductivity of polycrystalline material cannot be accurately modeled with conventional approaches for the thermal conductivity of bulk crystals. Here we adopt a model for the thermal conductivity in polycrystalline or composite materials based on the assumption of the phonon-hopping transport [4]. Under the framework of this model, the phonon thermal conductivity can be calculated as

\[
k = k_b T \int_0^{\theta} \frac{k_B B(x) \overline{S} \Phi}{h k_B^2 k_B a^2 d + k_B T_D B(x) \overline{S} \Phi} \, dx ,
\]

where \( h \) is the Planck’s constant, \( k_B \) is the Boltzmann’s constant, \( T_D \) is the Debye temperature, \( T \) is absolute temperature, \( a \) is the lattice constant, \( d \) is the average grain size. The parameter \( \overline{S} \) represents the mean area of the interface grain boundary and can be approximated as \( d^2 \). The disorder factor \( \Phi \) has been taken to be 0.87 for this work as prescribed in Ref. [4], where it was calculated in general case using the random number generator. The parameter \( t \) defines the transparency of the inter-grain boundary for the short wavelength phonons. Generally, it is difficult to determine \( t \) from the first principles since it depends on many factors and exact microstructure of the sample. In this work it is treated as a phenomenological parameter and its value is determined by fitting to the experimental data reported in Ref. [5]. The temperature dependence of the thermal conductivity is determined by the parameter \( B(x) \)

\[
B(x) = \frac{9}{2} \theta^4 x^4 e^x \left( \frac{x - 1}{\theta} \right)^2 ,
\]

where \( \theta = \frac{T}{T_D} \).

The regular thermal conductivity \( k_i \) of the constituent material that enters Eq. (1) is independent of any grain related parameters and given as

\[
k_i = \frac{1}{3} c_v \rho v l_{ph} ,
\]

where \( c_v \) is the specific heat, \( \rho \) is the mass density, \( v \) is the mean sound velocity of the phonons, and \( l_{ph} \) is the mean phonon’s free path in bulk material. We calculate the mean sound velocity from the equation
\[
\frac{3}{v^3} \times \frac{1}{v_L^3} + \frac{2}{v_T^3},
\]

where \(v_L\) and \(v_T\) are average longitudinal and average transverse sound velocities in GaN, respectively. The mean phonon free path can be expressed as

\[
l_{ph} = \frac{20T_m a}{\gamma T^2},
\]

where \(T_m\) is the melting point of the material and \(\gamma\) is the Gruneisen parameter.

It is important to note that GaN crystal has two lattice constants \(a_0 = 0.3189\text{nm}\) and \(c_0 = 0.5185\text{nm}\), and for this work the lattice constant in GaN is found as an average through the cubic root of the unit cell volume \(V_0\):

\[
a = \sqrt[3]{\frac{a_0 c_0 \sqrt{3}}{2}}.
\]

In Table I we summarized the material parameters used for modeling of the thermal conductivity of polycrystalline GaN.

**Table I. Material Parameters of GaN**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice constant (a_0, \text{nm}) [6]</td>
<td>0.3189</td>
</tr>
<tr>
<td>Lattice constant (c_0, \text{nm}) [6]</td>
<td>0.5185</td>
</tr>
<tr>
<td>Gruneisen parameter (\gamma) [1]</td>
<td>0.74</td>
</tr>
<tr>
<td>Longitudinal sound velocity (v_L, \text{cm/s}) [6]</td>
<td>(6.56 \times 10^5)</td>
</tr>
<tr>
<td>Transverse sound velocity (v_T, \text{cm/s}) [6]</td>
<td>(2.68 \times 10^5)</td>
</tr>
<tr>
<td>Debye temperature (T_D, K) [7]</td>
<td>600</td>
</tr>
<tr>
<td>Melting point (T_m, K) [8]</td>
<td>2227</td>
</tr>
<tr>
<td>Mass density (\rho, \text{g/cm}^3) [7]</td>
<td>6.15</td>
</tr>
<tr>
<td>Specific heat (c_V, J/(\text{gK})) [7]</td>
<td>0.49</td>
</tr>
</tbody>
</table>

**III. SIMULATION RESULTS**

Using material parameters from Table I and Eqs. (1-3) we simulated thermal conductivity in polycrystalline GaN. The average grain size was assumed to be 50 nm – 70 nm, which is consistent with experimental observations reported in Ref. [5]. Figure 1 shows the thermal conductivity as a function of temperature for three very different
values of the phonon transparency parameter $t$ and the grain size $d=50$ nm. The high value of the transparency parameter corresponds to the case when the material is “almost crystalline”. Thus, the dotted curve ($t=100$) displays a functional dependence typical of semiconductor crystals with a well-defined peak at low temperature and $1/T$ decrease at high temperature. The low value of the transparency parameter corresponds to the case when the material is “almost amorphous”. Correspondingly, the solid curve ($t=1$) shows the temperature dependence characteristic for amorphous materials. For intermediate values of the transparency parameter ($t=10-25$) the thermal conductivity is a weak function of temperature with values of approximately $0.4 \text{ W/cmK} - 0.9 \text{ W/cmK}$.

![Graph showing thermal conductivity of polycrystalline GaN](image)

Figure 1. Thermal conductivity of polycrystalline GaN as a function of temperature for different values of the inter-grain transparency parameter.

Recently reported measured thermal conductivity of polycrystalline GaN is $k = 0.8 \text{ W/(cm K)}$ at $T = 300$ K [5]. Using this data as a reference we found the value of the transparency parameter to be $t=25$ for a given material system and characteristic polycrystalline GaN grain size. Fitting the numeric data to the expression $k=A/T^\alpha$ over the range of temperatures from $300$ K to $1000$ K, we extracted the temperature dependence of the thermal conductivity. For the determined transparency parameter ($t=25$), the thermal conductivity $k$ is proportional to $1/T^{0.46}$. For the transparency parameter $t=10$, the thermal conductivity is proportional to $1/T^{0.26}$. This weak temperature
dependence of the thermal conductivity of polycrystalline GaN is in line with the experimentally determined dependence $\sim T^{-0.2}$. For crystalline GaN with high density of point defects and dislocations, we have previously determined that the thermal conductivity depends on temperature as $1/T^{d_{0.5}}$ [2, 9, 10]. For comparison, in high quality crystalline materials without many defects, the major thermal conductivity limiting mechanism at high temperature is phonon-phonon Umklapp scattering, which leads to the $1/T$ dependence on temperature.

IV. CONCLUSIONS

We presented preliminary results of simulation of the thermal conductivity in polycrystalline GaN. The calculation is based on the model for the phonon hopping transport and under the assumption that the phonon scattering at the grain boundaries is the major resistive mechanism. The extracted weak temperature dependence of the thermal conductivity, $T^{-0.46} - T^{-0.26}$, is in line with experimental data.

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