PHYSICAL REVIEW B **66**, 174301 (2002)

Lattice thermal conductivity in cubic silicon carbide

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(Received 20 May 2002; published 1 November 2002)

The lattice thermal conductivity of cubic silicon carbide is evaluated by means of a microscopic model considering the discrete nature of the lattice and its Brillouin zone for phonon dispersions and scattering mechanisms. The phonon Boltzmann equation is solved iteratively, with the three-phonon normal and umklapp collisions rigorously treated, avoiding relaxation-time approximations. Good agreement with the experimental data is obtained. Moreover, the role of point defects, such as antisites, on the lattice thermal conductivity is discussed.

DOI: 10.1103/PhysRevB.66.174301 PACS number(s): 66.70.+f, 63.20.Mt

Starting from 1960, thermal characterization of solids revealed that most of the high thermal conducting materials are adamantine (diamondlike) compounds such as diamond, SiC, AlN, GaN, Silicon, etc.[1] These compounds are used for compact semiconductor devices, where an efficient heat removal can be crucial to give good performances. To see if it is possible to increase the device substrate ability in the thermal management, experimental investigations have been recently done on some of these materials (diamond, silicon, and also germanium[2–7]) to establish the role on the phonon conductivity of defects, impurities, grain boundaries, and so on.

Good thermal conductors are important not only for the device itself, but also for the development of new components in the semiconductor processing equipments, as revealed by the market of SiC and AlN ceramics that registered a strong increase in past few years.[8] At present, silicon carbide is one of the most widely used ceramics for high thermal conductor applications, as well as for applications where strength and high mechanical stability are required.

Lattice conductivity of SiC in the chemical vapor deposition grade is around 300 $\mathrm{W\,m^{-1}\,K^{-1}}$ and 100 $\mathrm{W\,m^{-1}\,K^{-1}}$ in ceramics, at room temperature (see data from Insaco, Inc.[9] and from Saint-Gobain, Advanced Ceramics[10]): heat transport is lower than in diamond, the best heat conducting material, but of the same order as in copper. It can sound quite surprising but, in some cases, phonons are much more efficient to carry heat than electrons in metals.

Silicon carbide crystallizes in different polytypic forms: it occurs in cubic (β-SiC, also called 3C-SiC), but also in complex, long-range-ordered hexagonal and rhombohedral structures. First-principles investigations[11,12] of structural, lattice-dynamical, and electronic properties have been performed, with some attempts to explain the phenomenon of the polytypism,[13] and ‘‘*ab initio*’’ calculations were also made to obtain lattice properties.[14] The thermal conductivity was considered by means of a molecular-dynamics simulation[15] with an empirical potential (Tersoff model), obtained by matching the individual Tersoff models for Si and C.[16–18] The molecular-dynamics simulation gives good agreement with experimental data in the temperature range between 400 K and 1100 K.

In this paper, the β-SiC thermal conductivity is obtained by solving the phonon transport equation through an iterative procedure previously introduced for rare-gas solids[19,20] and then extended to diamondlike solids (Si, Ge, and diamond).[21,22] For these materials, the predicted temperature behavior of the thermal conductivity was found in excellent agreement with experimental data and a satisfactory explanation of the isotope scattering effect was obtained.

The interaction between atoms is expressed in terms of a pair potential with parameters obtained by fitting the experimental phonon spectrum. The iterative approach allows one to take into account the discrete nature of crystal lattice and its true Brillouin zone for the calculation of phonon dispersion and for the determination of three-phonon scattering processes. Moreover, the probability rates of various scattering mechanisms contributing to the thermal resistance is considered without the use of the relaxation-time approximation.

As we shall see, the calculation of thermal conductivity κ of β-SiC shows good agreement with experimental data. In the evaluation of κ the role of point defects, in particular antisites defects, will be specifically considered. Antisites produce a strong reduction in lattice heat transport and κ turns out to be only slightly depending on the temperature for high concentrations of defective lattice sites.

As previously done for Si, Ge, and diamond,[21,22] let us consider the phonon system for a cubic solid with a diamondlike lattice, with two atoms in the lattice cell with different masses. The elementary crystal excitation in the harmonic approximation is a phonon described by wave vector $\mathbf{q}$ and polarization index p. The frequency of the excitation will be indicated by $\omega_{\mathbf{q},p}$ and by $\boldsymbol{\epsilon}_{\mathbf{q}p,\mathbf{b}}$ the polarization vector associated to the vibration of the atom at the position $\mathbf{b}$ in the lattice cell situated at the position vector $\mathbf{l}$. In the case of diamondlike silicon carbide, vector $\mathbf{b}$ has only two possible determinations.

If N is the total number of cells in the crystal, the expansion of the displacement field $\boldsymbol{\eta}_{\mathbf{lb}}$ in terms of phonon absorption and creation operators $a_{\mathbf{q}p}$, $a^{\dagger}_{\mathbf{q}p}$, can be written in the form

$$\boldsymbol{\eta}_{\mathbf{lb}}=i\left(\frac{\hbar}{2M_bN}\right)^{1/2}\sum_{\mathbf{q}p}\frac{1}{\sqrt{\omega_{\mathbf{q}p}}}[\boldsymbol{\epsilon}^{*}_{\mathbf{q}p,\mathbf{b}}e^{-i\mathbf{q}\cdot\mathbf{l}}a_{\mathbf{q}p}-\boldsymbol{\epsilon}_{\mathbf{q}p,\mathbf{b}}e^{i\mathbf{q}\cdot\mathbf{l}}a^{\dagger}_{\mathbf{q}p}], \tag{1}$$

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where M_b is the atomic mass of $(\mathbf{l},\mathbf{b})$ site. This representation corresponds to that introduced by Srivastava.[23]

Using a pair potential $V(r)$, where r is the interatomic distance, one can easily expand function V in terms of the displacements $\boldsymbol{\eta}_{\mathbf{lb}}$, obtaining the second-order term of the potential energy of the interaction between two atoms at positions $(\mathbf{l},\mathbf{b})$ and $(\mathbf{l}',\mathbf{b}')$:

$$V^{(2)}_{\mathbf{lb},\mathbf{l'b'}}=\frac{1}{2}\{\gamma_{\mathbf{lb},\mathbf{l'b'}}\mathbf{\Delta}\cdot\mathbf{\Delta}+\beta_{\mathbf{lb},\mathbf{l'b'}}\,[(\mathbf{l}'-\mathbf{l}+\mathbf{b}'-\mathbf{b})\cdot\mathbf{\Delta}]^2\}, \tag{2}$$

where $\mathbf{\Delta}=\boldsymbol{\eta}_{\mathbf{l'b'}}-\boldsymbol{\eta}_{\mathbf{lb}}$ and the coefficients $\gamma_{\mathbf{lb},\mathbf{l'b'}}$, $\beta_{\mathbf{lb},\mathbf{l'b'}}$ are related to the first- and second-order derivatives of the potential. The coupling coefficients take values that will be denoted by γ and β, respectively, for atoms at the nearest-neighbor distance R and by γ' and β' for atoms at the next-nearest-neighbor distance R' (let us assume for γ',β' the same value for Si-Si and C-C interactions). In Ref. 21 adimensional parameters were introduced: $\rho=\gamma/(\beta R'^2),\rho'=\gamma'/(\beta R'^2)$. For the lattice constant of cubic SiC, the value 4.359×10^{-8} cm is assumed.

The parameters β, β', γ, and γ' are governing the equation of atomic motion and can be obtained by fitting the experimental phonon-dispersion curves. For the problem under consideration, that is the study of thermal conductivity, the use of a more sophisticated potential, such as a Tersoff potential, is not essential. The Tersoff potential is a pair potential with coefficients depending on the local environment[16] and is then fundamental to obtain reticular configurations and defect energies. For the thermal conductivity evaluation, the pair potential used in this paper is not less convenient than a Tersoff potential, due to the fact that, in both cases, adjustable parameters are introduced to fit the phonon-dispersion curves.

As in Ref. 21, the equation of motion can be solved to obtain phonon frequency and polarization vectors. The mass difference of atoms in the lattice cell produces an overall lowering of the acoustic-phonon branches. The pair potential alone is not able to give the splitting at $\mathbf{q}=\mathbf{0}$ of the optical modes and the raising of the longitudinal-optical (LO) mode frequency above that of the transverse-optical (TO) mode, since these effects are due to the long-range contribution of the Coulomb interaction.

The shift of LO mode is here considered as a perturbation in the phonon Hamiltonian, changing the LO frequency by a factor $\sqrt{\epsilon_o/\epsilon_\infty}$, where $\epsilon_o,\epsilon_\infty$ are the static and the high-frequency dielectric constants, as discussed by Born and Huang.[24] For β-SiC, $\epsilon_o=9.71$, $\epsilon_\infty=6.52$,[25] giving a shift of 22%, the same value that one can obtain by fitting the phonon-dispersion data of the LO branch.

In Fig. 1 the result of the calculation of phonon dispersions by means of the atomic motion equation is shown: the parameters are chosen to have the best possible agreement with the experimental data[26,27] and turn out to be $\rho=0.06$ and $\beta=4.6,\beta'=0.18$ (β,β' are in units of $10^{20}\,\mathrm{g\,cm^{-2}\,s^{-2}}$). The value of ρ' is assumed to be $\rho'=-\rho/8$, as was obtained in Ref. 21. The main role in the equation of motion is played by β and ρ, while β', ρ' slightly improve the fit to the experimental data. The assumption of a common parameter to account for the next-nearest-neighbor interactions, for any pair of atoms under consideration, is then justified.

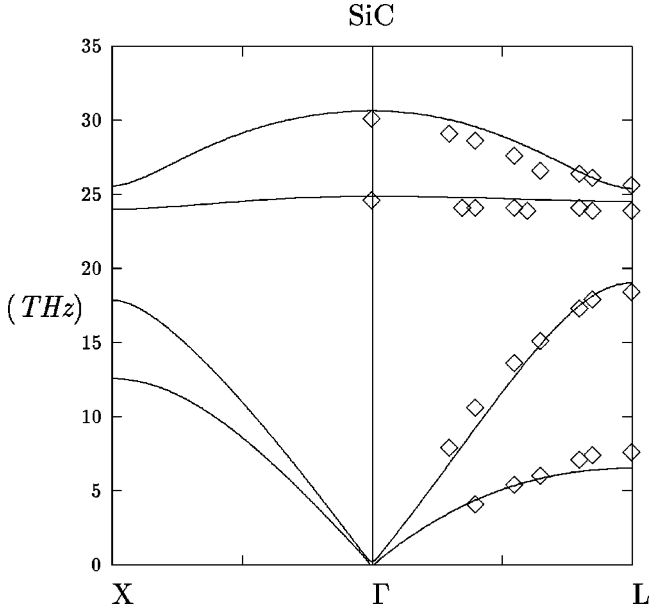

FIG. 1. Theoretical phonon-dispersion curves (continuous lines) for cubic SiC, in comparison with experimental data (Ref. 26).

In order to avoid the use of relaxation-time approximation and consider the discrete lattice nature and the true Brillouin zone, we introduce the third-order contribution of the interaction energy between the two reticular centers at $\mathbf{l},\mathbf{b}$ and $\mathbf{l}',\mathbf{b}'$:[19,20]

$$V^{(3)}_{\mathbf{lb},\mathbf{l'b'}}=\tfrac{1}{6}\,\alpha_{\mathbf{lb},\mathbf{l'b'}}\,[(\mathbf{l}'-\mathbf{l}+\mathbf{b}'-\mathbf{b})\cdot\mathbf{\Delta}]^3+\tfrac{1}{2}\,\beta_{\mathbf{lb},\mathbf{l'b'}}\,[(\mathbf{l}'-\mathbf{l}+\mathbf{b}'-\mathbf{b})\cdot\mathbf{\Delta}][\mathbf{\Delta}\cdot\mathbf{\Delta}] \tag{3}$$

where $\alpha_{\mathbf{lb},\mathbf{l'b'}}$ involves the third-order derivatives of the potential. By summing over all the lattice sites, the total anharmonic contribution $H^{(3)}$ to the crystal energy is obtained and the matrix elements $\langle q''p''|H^{(3)}|qp,q'p'\rangle$ and $\langle qp|H^{(3)}|q'p',q''p''\rangle$ can be evaluated. The probability rates connected with the above matrix elements will be denoted by $\mathcal{Q}^{q''p''}_{qp,q'p'}$, $\mathcal{Q}^{q'p',q''p''}_{qp}$, respectively. In the three-phonon processes, the phonon wave vector $\mathbf{q}$ belongs to the true Brillouin zone of the lattice and the momentum conservation is rigorously treated also in the umklapp case.

Considering only nearest-neighbor interactions in the evaluation of three-phonon scattering, the anharmonic dimensionless parameter $\varepsilon=-R'^2\alpha/\beta$ can be used. To estimate parameter ε it is necessary to know the Grüneisen constant γ of the material: in the case of β-SiC, a value of $\gamma=1.2$ at high temperatures, giving $\varepsilon=35$, can be deduced from Ref. 14.

To obtain the thermal conductivity, we linearize the Boltzmann equation for the phonon distribution. In terms of the deviation function $\psi_{\mathbf{q}p}$, linking the perturbed and unperturbed phonon distributions $n_{\mathbf{q}p}$ and n^o_{qp} in this manner

$$n_{\mathbf{q}p}=n^{o}_{qp}-\psi_{\mathbf{q}p}\frac{\partial n^{o}_{qp}}{\partial(\hbar\omega_{qp})}, \tag{4}$$

the linearized Boltzmann equation for a solid subjected to a thermal gradient $\boldsymbol{\nabla}T$ can be written in the following form:[28]

$$\begin{aligned}k_BT\ \ \mathbf{v}_{\mathbf{q}p}\cdot\boldsymbol{\nabla}T\frac{\partial n^{o}_{qp}}{\partial T}=&\sum_{\mathbf{q}'p'}\sum_{\mathbf{q}''p''}\mathcal{Q}^{\mathbf{q}''p''}_{\mathbf{q}p,\mathbf{q}'p'}[\psi_{\mathbf{q}''p''}-\psi_{\mathbf{q}'p'}-\psi_{\mathbf{q}p}]\\&+\frac{1}{2}\sum_{\mathbf{q}'p'}\sum_{\mathbf{q}''p''}\mathcal{Q}^{\mathbf{q}'p',\mathbf{q}''p''}_{\mathbf{q}p}[\psi_{\mathbf{q}''p''}+\psi_{\mathbf{q}'p'}\\&-\psi_{\mathbf{q}p}]+\sum_{\mathbf{q}'p'}\mathcal{Q}^{\mathbf{q}'p'}_{\mathbf{q}p}[\psi_{\mathbf{q}'p'}-\psi_{\mathbf{q}p}]\\&-\frac{1}{\tau_{qp}}\psi_{\mathbf{q}p}n^{o}_{qp}(1+n^{o}_{qp}),\end{aligned} \tag{5}$$

where the first and the second terms on the right-hand side describe three-phonon scattering processes, the third term is the elastic scattering due to impurities, and the fourth term provides a phenomenological description of boundary scattering in terms of relaxation times $\tau_{\mathbf{q}p}$. The phonon group velocity $\partial\omega_{qp}/\partial\mathbf{q}$ is denoted by $\mathbf{v}_{\mathbf{q}p}$.

An iterative procedure is used for solving the Boltzmann equation:[20,21] once $n_{\mathbf{q}p}$ is known, the heat current density

$$\mathbf{U}=\frac{1}{\Omega}\sum_{\mathbf{q}p}\hbar\omega_{qp}\mathbf{v}_{qp}n_{\mathbf{q}p} \tag{6}$$

is evaluated (Ω is the total volume of the crystal), and from the ith component of $\mathbf{U}$ with respect to the Cartesian reference frame

$$U_i=-\sum_j\kappa_{ij}\frac{\partial T}{\partial x_j} \tag{7}$$

the tensor representative of the thermal conductivity of the material κ_{ij}, is immediately obtained.

Parameters ρ, ρ', β, β', and ε are the only parameters that must be inserted in the calculation of the thermal conductivity: let us stress that all the parameters employed in the theory have been independently justified through the harmonic and anharmonic vibrational properties of the crystal, that is, phonon-dispersion experimental curves and Grüneisen parameter.

The thermal conductivity of the cubic SiC is shown in Fig. 2: it is in full agreement with the experimental conductivity values obtained in Refs. 29 and 30. If only three-phonon scattering mechanisms are considered, κ sharply increases at low temperatures (see curve *a* in Fig. 2). No difficulties are found in the evaluation of κ at low temperatures, while relevant problems are known to arise in the molecular-dynamics calculations.[15]

The relaxation-time approximation is avoided for the three-phonon scatterings but is introduced for boundary scattering in the form of $\tau_p=L/s_p$, where L represents a characteristic length in the sample,[28] and s_p the velocity of sound for a phonon with polarization index p.

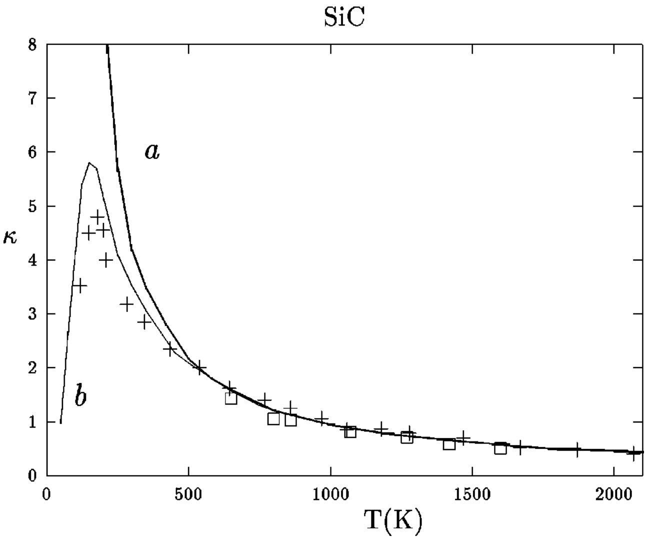

FIG. 2. Thermal conductivity (in W cm^{-1} K^{-1}) of cubic SiC, as a function of temperature, resulting from the present iterative calculation (continuous lines). Curve *a* represents the theoretical conductivity obtained when only three-phonon scattering processes are considered. Curve *b* is obtained including the presence of microcrystallites in the sample. Curves *a,b* are compared with experimental data of Taylor *et al.* (Ref. 29) (+) and of Senor *et al.* (Ref. 30) (□).

From the comparison of the theoretical calculations with the experimental data, we can see that a scattering mechanism different from three-phonon processes becomes important below 400 K. The origin of the mechanism can be viewed in the presence of microcrystallites, whose grain boundaries are scattering phonons in the experimental samples. As discussed by Ziman, a simple form of relaxation time, as the one used for scattering due to sample boundaries, can be introduced for the grain-boundary scattering. In Fig. 2, curve *b* represents the behavior of thermal conductivity with a relaxation time of the Ziman form: the value of L used to fit experimental data turns out to be ~ 2 μm.

The calculation of the grain-boundary effect used here can be only qualitative: as discussed in Ref. 31, the role of grain boundaries in diffracting phonons is much more complex, but the experimental data in the low-temperature region of SiC are really too poor for a reliable comparison.

The microscopic model used in the calculation of three-phonon scattering allows the evaluation of the role played by optical phonons, and in particular by the LO mode. In Table I, the values of κ are listed, referring to a calculation with all the acoustic- and optical-phonon modes included in the scattering mechanisms (first column κ_{all}). The other two columns in Table I show the results obtained considering (a) in the second column marked by κ_{ac+to}, phonons of acoustic and transverse optical modes, and (b) in the third column marked κ_{ac} only phonons in the acoustic modes. Let us note that the role of optical phonons is considerable at high temperatures.

Comparing the values of κ_{all} and κ_{ac+to}, one must conclude that the LO mode plays a certain role, in spite of its

TABLE I. Thermal conductivity of cubic silicon carbide resulting from the present iterative calculation. The First column lists the value of conductivity κ_{all} obtained considering all the phonon (acoustic and optical) modes. In the second column, the conductivity κ_{ac+to} is evaluated without considering in the calculation phonons of the LO mode. The last column gives κ obtained with only acoustic phonons present in the lattice. The values of κ are in W cm^{-1} K^{-1}. Note that the role of optical phonons is considerable at high temperatures.

$T(K)$	κ_{all}	κ_{ac+to}	κ_{ac}
800	1.35	1.61	2.48
1600	0.57	0.78	1.24

frequency shift. If the LO mode is considered without the Born shift, the thermal conductivity turns out to be furthermore reduced by $\sim 8\%$.

So far the discussion has been concerned with an ideal crystal and, for the low-temperature region, a crystal with grain boundary effect. Let us now discuss the role of point defects such as substitutional impurities. A point defect means first of all a mass difference in the lattice position where the defect is placed, giving a scattering probability rate of a phonon $\mathbf{q}p$ into a phonon $\mathbf{q}'p'$ of the form

$$\mathcal{P}_{\mathbf{q}p}^{\mathbf{q}'p'} = \frac{\pi}{2}\left(\frac{\Delta M}{M}\right)^2 \frac{1}{N^2}\,\omega_{\mathbf{q}p}\,\omega_{\mathbf{q}'p'}\,|\boldsymbol{\epsilon}_{\mathbf{q}p}\cdot\boldsymbol{\epsilon}_{\mathbf{q}'p'}|^2\,\delta(\omega_{\mathbf{q}p} - \omega_{\mathbf{q}'p'})\,n^o_{\mathbf{q}p}(1+n^o_{\mathbf{q}'p'}), \tag{8}$$

where ΔM is the mass variation. As discussed by Gurevich,[32] the defect gives also a potential-energy perturbation that can be included into Eq. (8) by the substitution

$$|\boldsymbol{\epsilon}_{\mathbf{q}p}\cdot\boldsymbol{\epsilon}_{\mathbf{q}'p'}| \rightarrow \left|\boldsymbol{\epsilon}_{\mathbf{q}p}\cdot\boldsymbol{\epsilon}_{\mathbf{q}'p'} + \frac{\Sigma}{\Delta M}\,\frac{\epsilon_i\epsilon_{i'}q_l q_{l'}}{\omega_{\mathbf{q}p}\omega_{\mathbf{q}'p'}}\right|^2, \tag{9}$$

where tensor Σ has dimensions of energy. The two terms are of comparable order provided ΔM is of the order of M and then the role of the point-defect perturbation can be evaluated, in a long-wave phonon approximation, as a contribution that turns out to be twice the contribution of the first term.

If the defects are assumed to be present in a fraction f_i of crystal sites, since the total number of atoms is twice the total number of cells N, there will be $2Nf_i$ centers producing elastic scattering in Eq. (5). Moreover, these defects are considered statistically distributed in both sites **b** of the lattice cell.

The probability rate can then be evaluated as in Ref. 21. In the calculation, a concentration of 0.5% point defects was assumed, each defect being considered as an antisite, where an Si atom is substituted by a C atom or vice versa. In Fig. 3, the result (curve b) of the present iterative procedure is shown with the data (points ×) obtained by Ju Li *et al.*[15] with molecular-dynamics (MD) simulations. The figure also reports, for comparison, the thermal conductivity for a perfect crystal obtained with the iterative procedure (curve a), and the data obtained with the MD simulation[15] (×). The experimental data of the sample without defects (+ and □ points) are also reproduced.

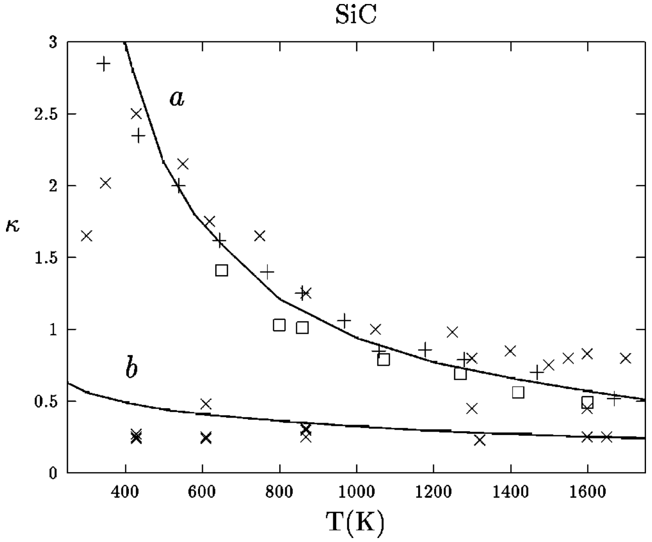

FIG. 3. Thermal conductivity (in W cm^{-1} K^{-1}) of cubic SiC, as a function of temperature. Curve a results from the present calculation in the case of a perfect crystal, whereas curve b is obtained for a crystal with antisite defects (0.5% of the lattice sites). Curves a,b are compared with experimental data (Refs. 29 and 30) (+,□) and with data obtained by Ju Li *et al.* (Ref. 15) by means of molecular-dynamics simulations (×).

Antitsite produce a strong reduction of κ and the lattice conductivity turns out to have only a slight temperature dependence: this is in agreement with the data obtained by Ref. 15 with MD simulation and with the experimental observations in irradiated specimens.[30,33,34]

In fact there is a difference between the defect microstructure assumed in calculations, where the defect distribution is thought to be a random distribution, and the defect arrangement in irradiation experiments.[15] First of all, in the scattering probability rate, point defects are considered as isolated defects at the same concentration throughout the entire range of temperatures. The defect microstructure in the actual irradiated specimens can be expected to vary appreciably with temperature. For a high defect concentration of 0.5%, defect clusters and void formation can occur as the temperature increases, particularly in the range above 1200 K. In Ref. 15, it is suggested that the role of crystal defects on thermal conduction will saturate; once this occurs, the defect distribution no longer matters for the behavior of κ.

The calculation of β-SiC thermal conductivity shows that the iterative approach to the Boltzmann equation is able to handle lattices with a complex structure. Through a limited number of parameters, determined by means of the experimental phonon dispersion of the crystal and by its Grüneisen constant, one is able to give a reliable calculation of thermal conductivity, where no approximations are introduced: this means that the model automatically includes both acoustic and optical modes with dispersion, correct umklapp processes, avoiding relaxation-time approximation for three-phonon scatterings.

In comparison with the MD simulations, the iterative approach does not show fluctuations in conductivity data at low temperatures, that is, for β-SiC, at room temperature. It is then possible to improve the investigations, by considering the role of extended defects (dislocations, grain boundaries, and so on), and to study other polytypes of silicon carbide.

As mentioned at the beginning of the paper, the use of high thermal conductivity materials is essential to thermal management in compact packaging systems, a key to further progress in this field. But high thermal conductivity polycrystalline materials are complex, and their optimization requires the study of thermal transport at different scales (including the effect of nanostructures and microstructures, which are present in the materials) to derive their macroscopic thermal behavior. The iterative technique can be a promising approach to the problem.

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