Thermal Models for Semiconductor Device Simulation

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Abstract—**We present models for the thermal conductivity and the specific heat applicable to all relevant diamond and zinc-blende structure semiconductors. They are expressed as functions of the lattice temperature and in the case of semiconductor alloys of the material composition.**

Keywords— **Electrothermal effects, Heating, Semiconductor device thermal factors, Simulation software.**

I. Introduction

SEVERAL applications of industrial interest employ devices with complex materials and structures operating in a wide temperature range. Accurate simulations save expensive technological efforts to obtain significant improvements of the device performance. For example, Heterojunction Bipolar Transistors (HBTs) attract much industrial interest nowadays because of their capability to operate at high current densities [1], [2]. Heat being generated at the heterojunctions cannot completely leave the device, especially in the case of III-V semiconductor materials. Therefore, significant self-heating takes place in the device, which leads to a change of the electrical device characteristics.

II. Self-heating simulation

The two-dimensional device simulator MINIMOS-NT [3] accounts for self-heating effects by solving the lattice heat flow equation (1) self-consistently with the energy transport equations. Finally, a system of six partial differential equations is being solved.

$$\mathrm{div}(\kappa_\mathrm{L} \cdot \mathrm{grad}\, T_\mathrm{L}) = \rho_\mathrm{L} \cdot c_\mathrm{L} \cdot \frac{\partial T_\mathrm{L}}{\partial t} - H \qquad (1)$$

In (1) T_L denotes the lattice temperature, t is the time variable, and H is the heat generation term. The coefficients are ρ_L, c_L, and κ_L, which denote the material's mass density, specific heat, and thermal conductivity, respectively. For different semiconductor materials proper models have to be used.

A. Mass Density Models

The values of the mass density of the basic semiconductor materials are well-known, and are used to model the values for compound materials. In the case of SiGe and ternary III-V alloys it is expressed by a linear change between the values of the basic materials A and B.

$$\rho^\mathrm{AB} = (1-x) \cdot \rho^\mathrm{A} + x \cdot \rho^\mathrm{B} \qquad (2)$$

The parameter values used in MINIMOS-NT are summarized in Table I.

TABLE I
Parameter values for mass density

Material	Value [g/cm^3]
Si	2.33
Ge	5.327
GaAs	5.32
AlAs	3.76
InAs	5.667
InP	4.81
GaP	4.138

B. Thermal Conductivity

The temperature dependence of κ_L of the basic semiconductor materials is modeled by a simple power law

$$\kappa_\mathrm{L}(T_\mathrm{L}) = \kappa_{300} \cdot \left(\frac{T_\mathrm{L}}{300\ \mathrm{K}}\right)^\alpha \qquad (3)$$

where κ_{300} is the value for the thermal conductivity at 300 K. This approximation is in good agreement with experimental data [4]-[7], as presented in Fig. 1 and Fig. 2 where comparisons between experimental data and the results obtained with our model are shown for the thermal conductivity at several temperatures in the range of interest (300 K – 800 K). The parameter values used are summarized in Table II.

TABLE II
Parameter values for thermal conductivity

Material	κ_{300} [W/K m]	α
Si	148	-1.65
Ge	60	-1.25
GaAs	46	-1.25
AlAs	80	-1.37
InAs	27.3	-1.1
InP	68	-1.4
GaP	77	-1.4

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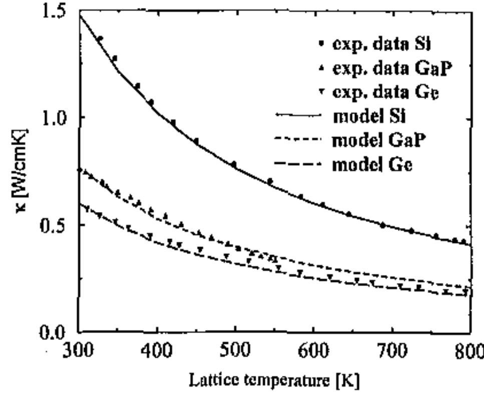

Fig. 1. Temperature dependence of the thermal conductivity. Comparison between experimental data and the model for Si, Ge, and GaP.

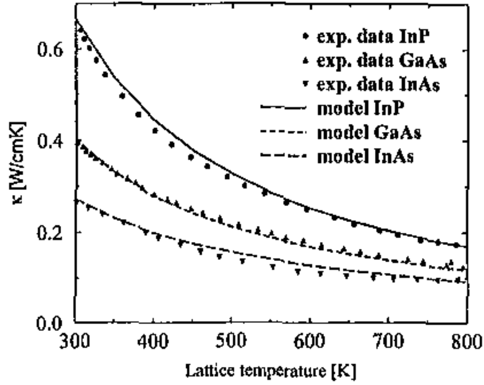

Fig. 2. Temperature dependence of the thermal conductivity. Comparison between experimental data and the model for InP, GaAs, and InAs.

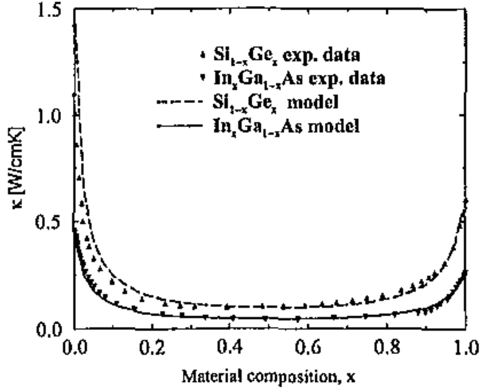

Fig. 3. Material composition dependence of the thermal conductivity. Comparison between experimental data and the model for SiGe and InGaAs.

In addition, the functional form given in (3) is easily integrated over temperature to obtain the lattice thermal flux density between two boxes which is defined by the lattice temperatures T_1 and T_2 of the respective box and is expressed by (4)

$$\int_{T_1}^{T_2} \kappa(T_L)\, dT_L = \frac{\kappa_{300}}{\alpha+1} \cdot \left[\left(\frac{T_2}{300\ \mathrm{K}}\right)^{\alpha+1} - \left(\frac{T_1}{300\ \mathrm{K}}\right)^{\alpha+1} \right]. \quad (4)$$

In the case of alloy materials $A_{1-x}B_x$ κ_L varies between the values of the basic materials (A and B). A harmonic mean is used to model κ_{300}. An additional bowing factor C is introduced in order to account for the drastic reduction of the thermal conductivity with the increase of material composition x. The temperature dependence factor α is linearly interpolated because insufficient experimental data at temperatures other than 300 K are available.

$$\kappa_{300}^{AB} = \frac{1}{\left(\frac{1-x}{\kappa_{300}^{A}} + \frac{x}{\kappa_{300}^{B}} + \frac{(1-x)\cdot x}{C}\right)} \quad (5)$$

$$\alpha^{AB} = (1-x)\cdot\alpha^{A} + x\cdot\alpha^{B} \quad (6)$$

The parameter values used in MINIMOS-NT are summarized in Table III. In Fig. 3 and Fig. 4 comparisons between experimental data from [5]-[10] and the results obtained with our model are shown for the thermal conductivity at 300 K.

TABLE III
PARAMETER VALUES FOR THERMAL CONDUCTIVITY

Material	C [W/K m]
SiGe	2.8
AlGaAs	3.3
InGaAs	1.4
InAlAs	3.3
InAsP	3.3
GaAsP	1.4
InGaP	1.4

C. Specific heat

For transient simulation with self-heating, the time-dependent term of (1) is discretized implicitly [12]:

$$\rho_L \cdot c_L \cdot \frac{\partial T_{L,n}}{\partial t} = \rho_L \cdot \bar{c}_L \cdot \frac{T_{L,n} - T_{L,n-1}}{\Delta t} \quad (7)$$

The parameter n denotes the corresponding time step. The temperatures $T_{L,n}$ and $T_{L,n-1}$ are also input parameters of the specific heat model (8). The function also requires the coefficients for the specific heat capacity of the considered material.

$$\bar{c}_L(\overline{T}) = c_{300} + c_1 \cdot \frac{\left(\frac{\overline{T}}{300\ \mathrm{K}}\right)^{\alpha} - 1}{\left(\frac{\overline{T}}{300\ \mathrm{K}}\right)^{\alpha} + \frac{c_1}{c_{300}}} \quad (8)$$

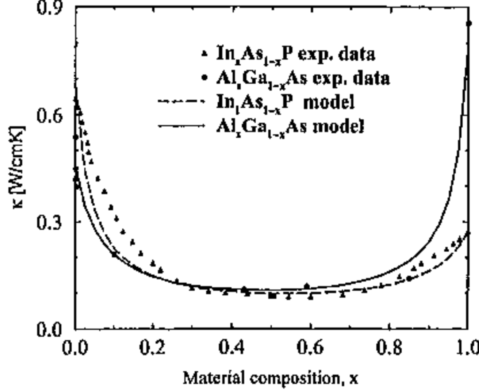

Fig. 4. Material composition dependence of the thermal conductivity. Comparison between experimental data and the model for InAsP and AlGaAs.

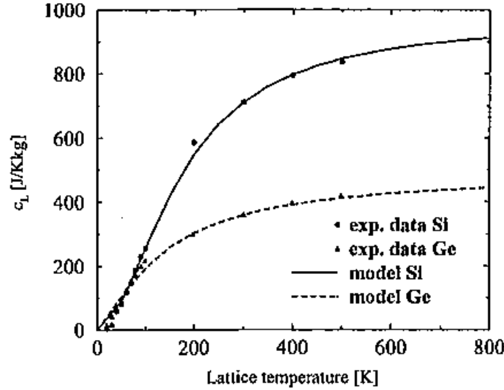

Fig. 5. Temperature dependence of the specific heat. Comparison between experimental data and the model for Si and Ge.

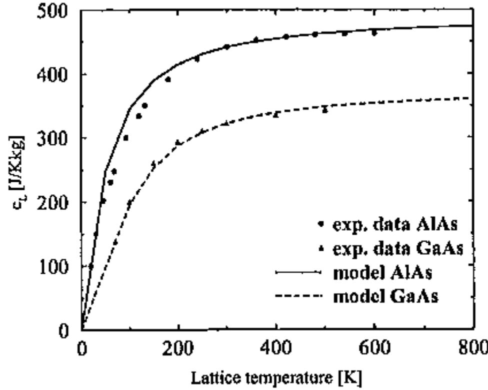

Fig. 6. Temperature dependence of the specific heat. Comparison between experimental data and the model for GaAs and AlAs.

$$\overline{T} = \frac{T_{L,n} + T_{L,n-1}}{2} \tag{9}$$

c_{300} is the value for the specific heat at 300 K [11]. The model is used for the basic semiconductor materials. We present in Fig. 5 and Fig. 6 comparison between experimental data and the results obtained with our model are for the specific heat. Note, the excellent agreement it gives in so wide temperature range (0 K – 800 K). The parameter values used are summarized in Table IV.

TABLE IV
PARAMETER VALUES FOR THE SPECIFIC HEAT

Material	c_{300} [J/K kg]	c_1 [J/K kg]	α
Si	711	255	1.85
Ge	360	130	1.3
GaAs	322	50	1.6
AlAs	441	50	1.2
InAs	394	50	1.95
InP	410	50	2.05
GaP	519	50	2.6

The specific heat capacity coefficients in the case of SiGe and ternary III-V compounds are expressed by a linear change between the values of the basic materials (A and B).

$$\bar{c}_L^{AB} = (1 - x) \cdot \bar{c}_L^A + x \cdot \bar{c}_L^B \tag{10}$$

The specific heat capacity is then expressed by (8).

III. Simulation Results

In particular the self-heating effects in an AlGaAs/InGaP/GaAs one-finger power HBT with emitter area of 90 μm^2 have been studied. A thermal contact at the substrate has been used. The thermal resistance contact model sets the contact temperature of the segment with a distributed lattice temperature attribute to a value which is calculated using the actual lattice temperature T_L, a specified contact temperature for the adjacent segment T_C, and a thermal resistance R_{Th}. The thermal heat flow density S_{T_L} at the contact boundary reads:

$$S_{T_L} = n \cdot \frac{T_L - T_C}{R_{Th}} \tag{11}$$

A measured value of about 400 K/W for R_{Th} has been used [1]. The resulting lattice temperature distribution over the device at $V_{CE} = V_{BE} = 1.6$ V is shown in Fig. 7.

The heat generated at the heterojunctions flows out of the device in the direction of the substrate heat sink. In the opposite direction the heat cannot leave the device and therefore the emitter finger is heated up significantly to more than 400 K. The simulation shown is of practical interest and demonstrates the need of using a thermal shunt at the emitter contact rather than reducing the substrate thickness.

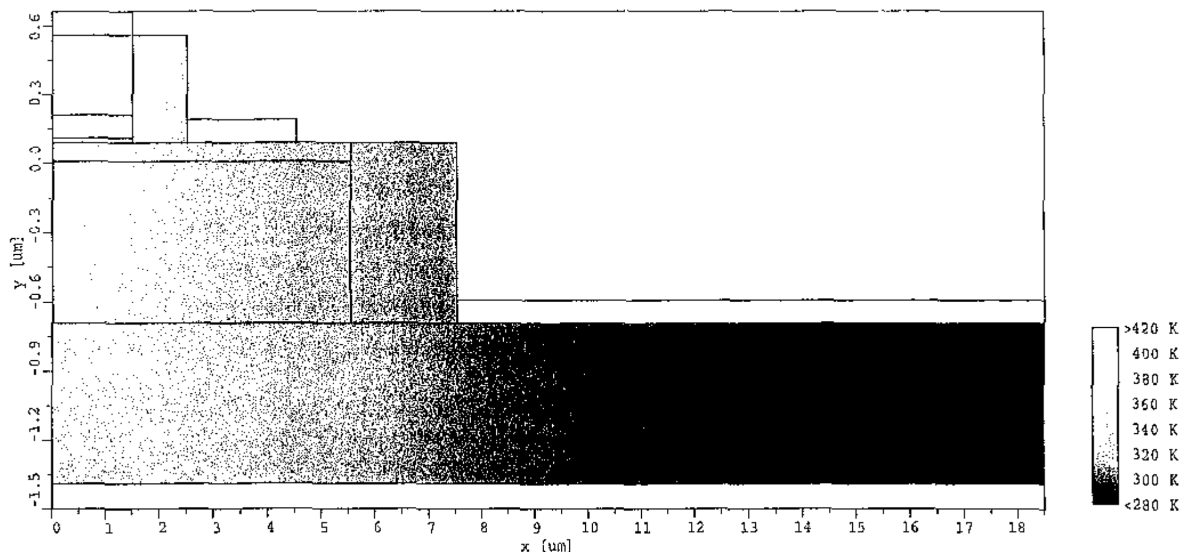

Fig. 7. Lattice temperature distribution in a power device at $V_{CE} = V_{BE} = 1.6$ V.

IV. Conclusions

We present thermal models for semiconductor device simulation valid in a wide temperature range and for all relevant semiconductors. Device simulation with self-heating was performed to proof the validity of the models.

Acknowledgments

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