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RIGOROUS THERMODYNAMIC TREATMENT OF HEAT GENERATION AND
CONDUCTION IN SEMICONDUCTOR DEVICE MODELING

G. Wachutka

Siemens AG, Research Laboratories, Munich, FRG

ABSTRACT

The influence of self-heating by power dissipation on the operation of semiconductor devices proves to be important not only in the area of power electronics, but also for VLSI devices. Hence, besides the carrier densities (or quasi-Fermi potentials, alternatively), temperature has to be included as additional dynamic state variable in the simulation of the electric and thermal behavior of such devices. However, up to now only heuristically introduced heat generation terms have been proposed as source in the heat conduction equation.

It is the scope of this paper to present a physically rigorous extension of the 'classical' (= isothermal) device equations to the case of variable (= space- and time-dependent) temperature which is based on the principles of irreversible thermodynamics (e.g., Onsager's relations and conservation of total energy) and, moreover, which is consistent with the models usually considered within the framework of the widely accepted isothermal drift-diffusion approximation. It turns out in the present theory that the heat sources can intuitively be interpreted as sum of the Joule heat and Thomson heat of both the electrons and the holes plus a term accounting for carrier recombination.

A critical comparison with previous work is made; it shows that, in the steady-state, some of the heuristic models for heat generation, thermal conductivity and heat capacity could indeed approximate the correct results within an error bound of 1...10%. In the transient regime, however, none of the models used hitherto proves to be applicable, in particular, if short pulse rise times of (< 10 ns) are attained.

INTRODUCTION

The modeling of semiconductor devices at isothermal conditions is essentially based on the continuity equations for electron and hole flow

$$(1) \quad \partial n / \partial t = -\text{div } \vec{j}_n + G - R$$

$$(2) \quad \partial p / \partial t = -\text{div } \vec{j}_p + G - R$$

(n, p: carrier concentrations; \vec{j}_n, \vec{j}_p : particle current densities of electrons and holes; G, R: generation- and recombination rates)

and Poisson's equation

$$(3) \quad \text{div}(\epsilon \vec{\nabla} \psi) = q (N_A^- - N_D^+ + n - p)$$

(ϵ : dielectric constant; ψ : electric potential; q: elementary charge; N_A^- , N_D^+ : concentrations of ionized acceptors and donors). In order to arrive at a closed system of equations, the particle fluxes \vec{j}_n and \vec{j}_p are commonly written as quasi-linear functions of driving forces in gradient form

$$(4) \quad \vec{j}_n = \mu_n n \vec{\nabla} \varphi_n$$

$$(5) \quad \vec{j}_p = -\mu_p p \vec{\nabla} \varphi_p$$

(μ_n, μ_p : mobilities; φ_n, φ_p : quasi-Fermi levels) with the driving potentials, φ_n and φ_p , being functions of the electric potential, ψ , and the carrier densities, n and p. In the case of a non-degenerate semiconductor, for instance, φ_n and φ_p are implicitly defined by Boltzmann relations

$$(6) \quad n = n_{ie} \exp((\psi - \varphi_n)/U_T)$$

$$(7) \quad p = n_{ie} \exp((\varphi_p - \psi)/U_T)$$

(n_{ie} : effective intrinsic concentration; $U_T = kT/q$: thermal voltage, with k: Boltzmann constant)

leading to the well-known representation of \vec{j}_n and \vec{j}_p as sum of a drift and a diffusion component.

In most cases, however, a semiconductor device cannot be operated at constant temperature due to self-heating by power dissipation. This phenomenon is not only characteristic of power electronics (see, e.g., Nakagawa and Ohashi, 1984), but also of growing importance in the area of VLSI and ULSI devices (Takacs and Trager, 1987). Hence, to account for non-isothermal effects in device modeling, a heat flow equation

$$(8) \quad c \cdot (\partial T / \partial t) = \text{div} (\kappa \vec{\nabla} T) + H$$

(c: heat capacity; κ : thermal conductivity; H: heat generation) must be added to the dynamic equations (1)-(2). Several proposals have been made for the heat generation model, H. So Gaur and Navon (1976) introduced H as Joule heat

$$(9) \quad H = \vec{j} \cdot \vec{E}$$

(\vec{j} : electric current density; \vec{E} : electric field), while Adler (1978) suggested

$$(10) \quad H = -\text{div} (E_C \vec{j}_n - E_V \vec{j}_p)$$

(E_C, E_V : band edges of conduction and valence band).

Chryssafis and Love (1979), on the other hand, recommended

$$(11) \quad H = q \cdot \text{div} (\varphi_n \vec{j}_n - \varphi_p \vec{j}_p)$$

Independently hereof, Elschner (1979) proposed

$$(12) \quad H = q \cdot \text{div} (\varphi_n \vec{j}_n - \varphi_p \vec{j}_p - \epsilon \gamma (\partial \vec{E} / \partial t))$$

Since all these models for H have been introduced by more or less heuristic reasoning based on ad-hoc assumptions, the obvious discrepancies are not very astonishing.

To clarify the situation, a rigorous thermodynamic approach to thermal generation is evidently required. It is the scope of this paper to present such an approach under the additional constraint that the extension to variable temperature should be consistent with the model equations (1)-(7) and should not violate any of the underlying postulates.

REVIEW OF THE BASIC ASSUMPTIONS

Before starting any attempt to extend the 'classical' device equations (1)-(5) to the non-isothermal case, we should clearly be aware of the underlying basic assumptions:

First of all, we deal with a phenomenological transport theory based upon the postulate that, even if we are far away from the thermodynamic equilibrium of the entire device, the electron and the hole subsystem, each of them per se, is locally in equilibrium; thus, at a position \vec{r} and a time t , any accessible state can be uniquely characterized by a temperature $T_n(\vec{r}, t)$ and $T_p(\vec{r}, t)$, respectively, and a quasi-Fermi level $\varphi_n(\vec{r}, t)$ and $\varphi_p(\vec{r}, t)$. In the same way, the states of the substrate lattice are uniquely determined by a lattice temperature $T_L(\vec{r}, t)$. The three subsystems are able to interchange energy with each other by various scattering mechanisms. So, for instance, energy can be transferred from the free carriers to the substrate via lattice scattering or (ionized) impurity scattering; by carrier-carrier scattering, energy flow between electrons and holes is enabled. Furthermore, there is also particle flow between the electron and hole system which is supported by various recombination and generation processes; since each of them involves energy exchange too, additional energy flows are induced (to the lattice, for example, by the SRH mechanism

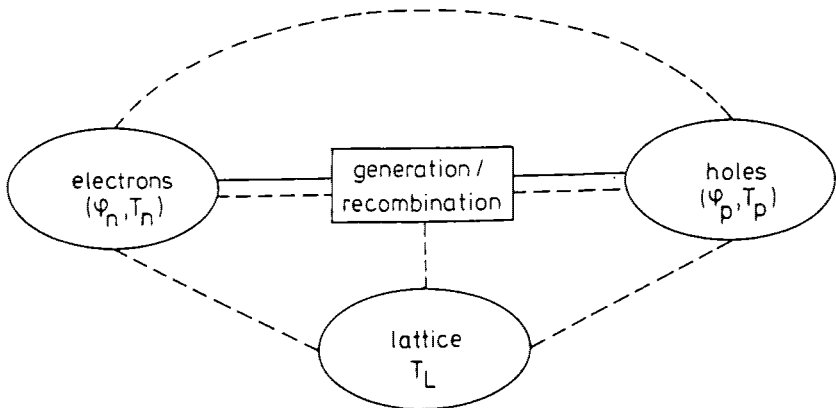


Fig. 1: Composite thermodynamic system comprising the subsystems of electrons, holes, and the substrate lattice (dashed lines denote energy (heat) flow, solid lines denote particle flow).

(Shockley and Read, 1952; Hall, 1952) and between the free carriers by Auger recombination). If radiative recombination and optical generation are neglected, the composite thermodynamic system comprising lattice, electrons, and holes (cf. fig. 1) is closed with respect to both particle and energy flow; hence, particle conservation (eqs. (1)-(2)) and energy conservation (eq. (15) in the next section) are valid.

Second, by omitting all hot carrier effects, we arrive at the postulate that the electrons and the holes are in thermal equilibrium with the lattice. Thus the electron and hole temperatures, $T_n(\vec{r}, t)$ and $T_p(\vec{r}, t)$, are set equal to the substrate temperature, $T_L(\vec{r}, t)$, which under isothermal conditions is equal to a constant T . Hence, solely the quasi-Fermi levels, $\varphi_n(\vec{r}, t)$ and $\varphi_p(\vec{r}, t)$, are left as dynamic variables; within the framework of the commonly used drift-diffusion approximation (see, e.g., Bonč-Bruevič and Kalašnikov, 1982), their spatial gradients, $\vec{\nabla}\varphi_n$ and $\vec{\nabla}\varphi_p$, are the forces driving the particle currents \vec{j}_n and \vec{j}_p , respectively (cf. eqs. (4)-(5)).

Third, to obtain a closed system of dynamic equations for φ_n and φ_p (or, equivalently, for the carrier concentrations n and p), we need to specify in which way φ_n and φ_p depend on n and p . Usually, this is done by introducing Fermi statistics (or, as approximation, Boltzmann statistics) and by assuming that the electric energy of the composite system is of purely electrostatic nature. In this way, each of the quasi-Fermi levels may be written as the sum of an electric potential ψ and a chemical potential. While the latter is a local function of the carrier densities and temperature, the electric potential depends non-locally on the carrier distributions $n(\vec{r}, t)$ and $p(\vec{r}, t)$ via Poisson's equation (3). Note that ψ is not a dynamic variable, but only an auxiliary quantity which couples the dynamic variables at a position \vec{r}' to those at a position \vec{r} quasi-statically (i.e. at the same time t) via an integral operator (= inverse Laplacian). Hence, the above assumptions do evidently not allow for electric fields which rapidly vary with time (and thus contradict Elschner's (1979) derivation of the total power loss density in semiconductors).

In the case of a non-degenerate semiconductor, the quasi-Fermi levels are easily calculated by inverting eqs. (6)-(7):

$$(13) \quad \varphi_n = \psi - U_T \ln(n/n_{ie})$$

$$(14) \quad \varphi_p = \psi + U_T \ln(p/n_{ie})$$

In the sequel, we will make use of these relations, whenever an explicit functional form for φ_n and φ_p is required (e.g., for the estimation of magnitudes).

CONSISTENT EXTENSION OF THE CLASSICAL SEMICONDUCTOR EQUATIONS TO VARIABLE TEMPERATURE

To be consistent with the isothermal device equations, we adhere to all the assumptions in the foregoing paragraph, with the sole exception of constant temperature. Instead, we regard temperature now as additional dynamic variable which may be position- and time-dependent: $T = T(\vec{r}, t)$. In order to obtain a dynamic equation for T , we calculate the total differential energy density du_{tot} and the total energy flux \vec{J}_{tot}^u of the composite system of lattice and carriers, with n , p , and T being chosen as independent dynamic variables. Then, making use of the principle of energy conservation,

$$(15) \quad \partial u_{\text{tot}} / \partial t + \text{div } \vec{J}_{\text{tot}}^u = 0$$

we will arrive at a partial differential equation for T , which completes the dynamic system (1)+(2).

To begin with, the phenomenological current relations (4)-(5) have to be supplemented by an additive term proportional to the gradient of T which acts as additional driving force (see, e.g., Callen, 1960):

$$(16) \quad \vec{J}_n = \mu_n n \cdot (\vec{\nabla} \varphi_n - P_n \vec{\nabla} T)$$

$$(17) \quad \vec{J}_p = -\mu_p p \cdot (\vec{\nabla} \varphi_p + P_p \vec{\nabla} T)$$

The coefficients P_n and P_p are the thermoelectric powers associated with the electron and hole system, respectively, and represent new model quantities.

Similar to the particle fluxes, the heat current densities of the carrier subsystems are linear combinations of the gradient of the respective quasi-Fermi potential and the temperature gradient:

$$(18) \quad \vec{j}_n^Q = n(q\mu_n P_n T \vec{\nabla} \varphi_n - (\lambda_n/T) \vec{\nabla} T)$$

$$(19) \quad \vec{j}_p^Q = -p(q\mu_p P_p T \vec{\nabla} \varphi_p + (\lambda_p/T) \vec{\nabla} T)$$

Note that not all kinetic coefficients arising in eqs. (16)-(19) are independent: As a consequence of Onsager's fundamental reciprocity theorem (Onsager, 1931), the thermoelectric powers determine not only the particle flow due to a temperature gradient, but also the heat flow due to a gradient of the quasi-Fermi levels. Through eqs. (18)-(19), therefore, solely λ_n and λ_p enter into the theory as new quantities. Instead of these, usually the thermal conductivities of the electron gas and the hole gas,

$$(20) \quad \kappa_n := n((\lambda_n/T) - q\mu_n P_n^2 T)$$

$$(21) \quad \kappa_p := p((\lambda_p/T) - q\mu_p P_p^2 T)$$

are introduced as independent model quantities, because they are easier accessible in theory and experiment.

Since heat transport in the lattice subsystem does not involve any particle fluxes, the heat current density of the lattice is proportional merely to $\vec{\nabla} T$:

$$(22) \quad \vec{j}_L^Q = -\kappa_L \vec{\nabla} T$$

where κ_L denotes the thermal conductivity of the substrate lattice.

The energy current density of each subsystem is the sum of heat flux plus the product of particle flux multiplied by the respective electrochemical potential; therefore the total energy current density reads:

$$(23) \quad \vec{j}_{\text{tot}}^u = -\kappa_L \vec{\nabla} T + \vec{j}_n^Q - q\varphi_n \vec{j}_n + \vec{j}_p^Q + q\varphi_p \vec{j}_p$$

Next, let us turn to the calculation of the differential energy densities: For the lattice, we have simply

$$(24) \quad du_L = c_L dT$$

with c_L being the heat capacity of the lattice. By applying the usual formalism of classical thermodynamics (e.g., Maxwell's relations), the energy densities of electrons and holes, respectively, can be represented in the differential form

$$(25) \quad du_n = c_n dT + q[T(\partial \varphi_n / \partial T)_{n,p} - \varphi_n] dn$$

$$(26) \quad du_p = c_p dT - q[T(\partial \varphi_p / \partial T)_{n,p} - \varphi_p] dp$$

Here, c_n and c_p are the heat capacities of the electron gas and hole gas, respectively; $(\partial / \partial T)_{n,p}$ stands for the partial derivative with respect to T at constant n and p . The second terms in (25)-(26) account for the fact that any change in the carrier concentrations (at constant temperature) results in a certain amount of energy interchanged between the constituent subsystems.

Inserting

$$(27) \quad du_{\text{tot}} = du_L + du_n + du_p$$

and \vec{j}_{tot}^u (cf. eq. (23)) into (15) yields the following 'heat conduction equation':

$$(28) \quad c_{\text{tot}} \cdot (\partial T / \partial t) = \text{div} (\kappa_{\text{tot}} \vec{\nabla} T) + H$$

where $c_{\text{tot}} = c_L + c_n + c_p$ is the total heat capacity, $\kappa_{\text{tot}} = \kappa_L + \kappa_n + \kappa_p$ is the total thermal conductivity, and

$$(29) \quad H = q \vec{j}_n^2 / (\mu_n n) + q \vec{j}_p^2 / (\mu_p p) + \\ + q(R-G)[T(\partial \varphi_n / \partial T)_{n,p} - \varphi_n - T(\partial \varphi_p / \partial T)_{n,p} + \varphi_p] + \\ + qT[(\partial \varphi_n / \partial T)_{n,p} - P_n] \cdot \text{div} \vec{j}_n - qT[(\partial \varphi_p / \partial T)_{n,p} + P_p] \text{div} \vec{j}_p - \\ - qT(\vec{j}_n \cdot \vec{\nabla} P_n + \vec{j}_p \cdot \vec{\nabla} P_p)$$

is a quantity which will be discussed in the next section.

Here, only the contributions of electrons and holes to the total heat capacity and thermal conductivity shall briefly be estimated: Assuming parabolic energy bands, we deduce from the free electron heat capacity that $c_n/c_L < 1\%$ and $c_p/c_L < 1\%$ if

only $n < 10^{21} \text{cm}^{-3}$ and $p < 10^{21} \text{cm}^{-3}$, respectively. If we furthermore suppose that mobility and thermal conductivity of the carriers obey a Wiedemann-Franz law, we obtain $\kappa_n / \kappa_L < 1 \%$ and $\kappa_p / \kappa_L < 1 \%$ for carrier concentrations less than 10^{19}cm^{-3} . In the case that the carrier densities should exceed this number, heavy doping effects on the lattice conductivity κ_L have also to be taken into account, and the experimental data (Maycock, 1967) indicate that the latter is dominant.

DISCUSSION OF THE THERMAL GENERATION TERM

The stationary case

In the steady-state, $\text{div } \vec{j}_n$ and $\text{div } \vec{j}_p$ in the third line of eq. (29) can be substituted by the generation/recombination rate G-R, and thus the heat source term H may be rewritten as

$$(30) \quad H = q \vec{j}_n^2 / (\mu_n n) + q \vec{j}_p^2 / (\mu_p p) + \\ + q(R-G) [\varphi_p - \varphi_n + T(P_n + P_p)] - qT(\vec{j}_n \vec{\nabla} P_n + \vec{j}_p \vec{\nabla} P_p)$$

Evidently the first two terms are the Joule heat of electrons and holes, the third one is the recombination heat, and the fourth one is known as Thomson heat (see, e.g., Callen, 1960). Except that the thermoelectric powers P_n and P_p appear in (30), it is in agreement with the results of Elschner (1979) and Chryssafis and Love (1979), when specialized to steady-state conditions. To estimate the corrections induced by P_n and P_p , we concentrate on the recombination heat, because here the major effect is to be expected. Theoretical investigations (Stratton, 1972; Bonč-Bruevič, 1982; Dorkel, 1983) predict $P_n T$, $P_p T \approx (0.5 \dots 5) U_T$; the experimental findings (Herring, 1958) are about $17 \cdot U_T$ (at 300 K). So $P_n T$ and $P_p T$ are not unlikely to exceed $\varphi_p - \varphi_n$ in (30) and, therefore, must not be neglected if the recombination heat becomes comparable with or much greater than the Joule heat. That such situations may occur has clearly been demonstrated by computer simulations (Elschner, 1979).

The transient case

In contrast to the steady-state, it is unfortunately not possible to eliminate the $\text{div } \vec{j}_n$ and $\text{div } \vec{j}_p$ terms in eq. (29) simply by inserting the particle continuity equations (1)-(2), because then the time-derivates of the carrier concentrations would appear on the right-hand side of (28). On the other hand, if we make use of the current relations (16) and (17) to evaluate $\text{div } \vec{j}_n$ and $\text{div } \vec{j}_p$, we obtain second order derivatives with respect to position which structurally belong to the elliptic part of the parabolic operator associated with the system (1)+(2)+(28). Hence, it seems most appropriate to rewrite (28) in divergence form

$$(31) \quad c_{\text{tot}} \cdot (\partial T / \partial t) = \text{div} (a_{TT} \vec{\nabla} T + a_{Tn} \vec{\nabla} \varphi_n + a_{Tp} \vec{\nabla} \varphi_p) + H'$$

with the modified source term

$$(32) \quad H' = q \vec{j}_n \vec{\nabla} \varphi_n - q \vec{j}_p \vec{\nabla} \varphi_p + \\ + q(R-G) [T(\partial \varphi_n / \partial T)_{n,p} - \varphi_n - T(\partial \varphi_p / \partial T)_{n,p} + \varphi_p] - \\ - \vec{j}_n \vec{\nabla} [qT(\partial \varphi_n / \partial T)_{n,p}] + \vec{j}_p \vec{\nabla} [qT(\partial \varphi_p / \partial T)_{n,p}]$$

and the coefficients

$$(33) \quad a_{TT} = \kappa_{\text{tot}} + q\mu_n n T P_n [P_n - (\partial \varphi_n / \partial T)_{n,p}] + \\ + q\mu_p p T P_p [P_p + (\partial \varphi_p / \partial T)_{n,p}]$$

$$(34) \quad a_{Tn} = -q\mu_n n T \cdot [P_n - (\partial \varphi_n / \partial T)_{n,p}]$$

$$(35) \quad a_{Tp} = q\mu_p p T \cdot [P_p + (\partial \varphi_p / \partial T)_{n,p}]$$

Note that H' is not the total thermal generation rate, because the flux under the div -operator is not the total heat current density.

For a more detailed interpretation of H' , we must specify the model for φ_n and φ_p . For the sake of simplicity, let us use eqs. (13)-(14) here, with n_{ie} being the intrinsic concentration of an idealized semiconductor (having parabolic energy

bands with constant effective masses); the extension to the general case is straightforward. Differentiating eqs. (13)-(14) with respect to T yields

$$(36) \quad T(\partial\varphi_n/\partial T)_{n,p} = T(\partial\psi/\partial T)_{n,p} + \varphi_n - \psi + 3/2 U_T + E_g/(2q)$$

$$(37) \quad T(\partial\varphi_p/\partial T)_{n,p} = T(\partial\psi/\partial T)_{n,p} + \varphi_p - \psi - 3/2 U_T - E_g/(2q)$$

(E_g denotes the band gap).

In the case of completely ionized donors and acceptors, the electric potential ψ does not depend on temperature; this supposed, we are able to continue the evaluation of H' :

$$(38) \quad H' = \vec{j} \cdot \vec{E} + (R-G)(E_g + 3kT) - (\vec{j}_n + \vec{j}_p)(3/2 k \vec{\nabla} T + 1/2 \vec{\nabla} E_g)$$

(\vec{j} : electric current density; \vec{E} : electric field)

and arrive at a very attractive result: The first term is the classical power loss in an isothermal unipolar conductor, while the second one accounts for the energy exchange with the lattice through recombination or generation of electrons and holes whose energy is $3/2 kT$ above the conduction band edge or $3/2 kT$ below the valence band edge, respectively (in exact agreement with the thermal average values!). The third term contributes corrections for a non-constant temperature distribution and variations of the band edges.

It is interesting to consider (38) at steady-state conditions; in this special case, H' may be written as

$$(39) \quad H' = - \operatorname{div} [(E_C + 3/2kT)\vec{j}_n - (E_V - 3/2kT)\vec{j}_p]$$

which, apart from the energy shifts $\pm 3/2 kT$, coincides with the formulation by Adler (1978). Therefore, his approach does not necessarily contradict that of Chryssafis and Love (1979), if only the correctly associated energy flux is used in the (stationary!) heat conduction equation.

Let us now briefly estimate the importance of the terms which, in addition to $\kappa_{\text{tot}} \vec{\nabla} T$, appear under the div-operator in eq. (31). By means of (36)-(37) we conclude that the range of $qT(\partial\varphi_n/\partial T)$ and $qT(\partial\varphi_p/\partial T)$ is on the scale of the band

gap E_g ; therefore, apart from the above discussed effects induced by the thermopowers, the non-diagonal terms $a_{Tn} \vec{\nabla} \varphi_n$ and $a_{Tp} \vec{\nabla} \varphi_p$ may be of the order of magnitude

$(E_g/2) |\vec{j}| \approx 0.5 \text{ VAc}^{-2} |\vec{j}| \text{ cm}^2/\text{A}$, while $\kappa_{\text{tot}} \vec{\nabla} T$ amounts to $|\kappa_{\text{tot}} \cdot \vec{\nabla} T| \approx 1.5 \text{ VAc}^{-2} |\vec{\nabla} T| \text{ cm/K}$. As has been demonstrated by Takacs and Trager (1987), either of these contributions will become dominant in VLSI devices, and hence each of the coupling coefficients a_{TT} , a_{Tn} , and a_{Tp} has to be carefully evaluated.

Moreover, by comparing (29) with (30) we conclude that the additional energy exchange due to the variation of the carrier concentrations with time in the transient regime is of the magnitude $(E_g/2)(\partial n/\partial t + \partial p/\partial t)$. It is easily shown that this quantity may largely exceed the Joule heat if pulse rise times of less than 10 ns are attained. Consequently, it is not allowed to extrapolate from the stationary thermal generation term (30) to the transient case.

RESUME

A physically rigorous extension of the isothermal semiconductor device equations to non-isothermal conditions has been formulated. It has been demonstrated that temperature may be included in the device dynamics as additional state variable without violating any of the basic assumptions underlying the isothermal case and without introducing inconsistencies with the models based on the isothermal drift-diffusion approximation. The given extension is also in accordance with the laws of phenomenological thermodynamics.

In the steady-state, the present theory leads to a classical heat conduction equation with a thermal generation term which is composed of the Joule heat and Thomson heat of electrons and holes plus a contribution accounting for recombination heat. Within certain limits, the result of the rigorous approach confirms the heuristic expressions given by Elschner (1979) and Chryssafis and Love (1979) as good approximations.

In the transient regime, we arrive at a heat conduction equation in generalized form involving each of the gradients of the quasi-Fermi potentials and of temperature as driving forces for heat flow. For non-degenerate semiconductors, the heat source term consists of isothermal Joule heat and isothermal recombination heat plus corrections for variable temperature

and variable band edges; when specialized to steady-state conditions, it is approximated by Adler's (1978) ansatz. However, some a-priori estimates indicate that none of the above cited models for thermal generation is applicable in the transient case.

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