



# Self-heating in semiconductors: A comparative study



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## ABSTRACT

A new expression for the source term  $H$ , in the heat flow equation is developed for bipolar semiconductors. This term consists of heat generated by carrier-lattice collisions, recombination of electrons and holes, and other processes. The expression allows self-consistent calculations of self-heating in any device. The derivation is based on thermoelectric concepts. There exists several expressions for  $H$  in the general literature for calculating the temperature field, and the presently developed one is compared with the older ones. Discrepancies exist between all of the formulas and reasons for them are given.

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## 1. Introduction

The calculation of self-heating in semiconductors has been continuously refined over the past 50 years. Though not a review paper, we continue the trend and develop a new equation for the generation of heat in a semiconductor when both electrons and holes contribute to the total current at the same point. Here we use the extended Drift-Diffusion approach along with thermoelectric concepts.

It is important to determine the temperature map in a semiconductor for obvious reasons; and especially for devices used in high temperature applications. For example, Sheng [1] has stated the maximum temperature permitted in a typical SiC JFET could be less than 200 °C; a junction above this may self-destruct due to thermal run-away. Thus a numerical simulation should be able to determine the junction temperature for a particular design rather accurately. Also since most of the parameters defining a semiconductor depend on temperature; these dependencies must be modeled if good accuracy is desired.

The calculation of the temperature depends on the correct form for the heat source term  $H$ . The basic semiconductor system is complex in that one deals with three interacting systems; the electrons, holes, and the lattice. Several equations for  $H$  have been developed and they are used in commercial simulators. However they show discrepancies which are not small. The development of  $H$  depends on careful bookkeeping of energy;

however, the bookkeeping of energy (for single carrier material) is not clear, as stated by Mahan [2]. The terms total energy, internal energy, heat flux vector, heat flow, energy flux vector, heat vector, thermal current density, and so forth; share the same group of symbols along with different definitions. These alternative approaches make the area of study confusing. Harman and Honig (H & H) [3] on pages 28, 29, 31, 32, 40, and 41 of their text discuss some of the errors in the thermoelectric field concerning the vectors  $\mathbf{J}_E$ ,  $\mathbf{J}_S$ ,  $\mathbf{J}_Q$  the energy flux vector, entropy flux vector, and the thermal-energy flux vector or thermal current density, respectively. On page 32 they state “Erroneous claims to the contrary have appeared in the literature when writers failed to distinguish between  $\mathbf{J}_Q$  and  $\mathbf{J}_E$ .”

Our approach to determine  $H$  is as follows. From general heat flow theory [4]

$$\nabla \cdot \mathbf{q} + \partial U / \partial t = \partial Q / \partial t \quad (1)$$

where  $\mathbf{q}$  is the rate heat is conducted across a unit surface.  $U$  is the internal energy per unit volume, and  $Q$  is the heat generated per unit volume. As you can see,  $\partial Q / \partial t = H$ , but we use  $H$  since the symbol  $Q$  has several meanings or interpretations in the literature. For the special case when  $\mathbf{q} = -\kappa \nabla T$ ,  $\mathbf{q}$  is called the conduction of heat between planes at different temperatures. Here  $\kappa$  is the thermal conductivity. The term  $\partial U / \partial t = \rho' C \partial T / \partial t$ , where  $\rho'$  and  $C$  are the mass density and specific heat per unit mass of the solid. For the case when no energy storage exists (when  $\partial U / \partial t = 0$  in the volume considered) and therefore all generated heat flows into the surroundings, we have

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$$\nabla \cdot \mathbf{q} = \partial Q / \partial t$$

A type of volume heat generation (for a single carrier case) is Joule heating for which  $\partial Q / \partial t = \rho J^2 = H'$ , where  $\mathbf{J}$  is the electric current density, and  $H'$  is the heat source term ( $\text{W}/\text{m}^3$ ) in this case. If one assumes Ohmic conduction, then  $\rho J^2$  may be written as  $\mathbf{J} \cdot \mathbf{E}$  where  $\mathbf{E}$  is the electric field.

$$\nabla \cdot \mathbf{q} = \mathbf{J} \cdot \mathbf{E} = H' \quad (2)$$

For the general case of a single charge carrier type (normally electrons), the thermal current and electric current densities may be written as [5,6]

$$\mathbf{q} = -\kappa \nabla T + \Pi \mathbf{J} \quad (3)$$

$$\mathbf{J} = -\sigma \nabla V - \alpha \nabla T \quad (4)$$

where  $\mathbf{J}$ ,  $\Pi$ ,  $V$ ,  $\sigma$ ,  $\alpha$  are the electric current density, Peltier coefficient, electrostatic potential, conductivity, and Seebeck coefficient, respectively. Inspection of these equations shows  $\mathbf{q}$  (in general) depends on gradients of both temperature and potential. Inserting (3) into (2) yields

$$\nabla \cdot (-\kappa \nabla T) + \nabla \cdot (\Pi \mathbf{J}) = H'$$

After rearranging we write (assume  $\kappa$  is a constant)

$$-\kappa \nabla^2 T = H \quad (5)$$

where  $H = H' - \nabla \cdot (\Pi \mathbf{J})$ . Thus  $H$  will denote terms that originate from the general  $\mathbf{q}$  term and for terms from the right side of Eq. (1). For example, another term we could place on the right hand side is the 'Thomson heat', which may be represented by  $-\mathbf{T} \mathbf{J} \cdot \nabla S$ , [2]. However in [2] the current density is represented by  $\mathbf{J} = -\sigma \nabla (\underline{\mu}/e) - \sigma \nabla T$ . Notice the changes in the definition for  $\mathbf{J}$  from that in Eq. (4). While  $S = \alpha$  is obvious, the difference in electrostatic potential and the  $\underline{\mu}/e$  term is not trivial. The term  $\underline{\mu}$  is the electrochemical potential. This illustrates some of the problems stated earlier concerning confusing notations, terminology, actual errors, and perhaps typos. One problem with the above statements is the assumption that we can write  $\rho J^2 = \mathbf{J} \cdot \mathbf{E}$ . The problem we run into is the fact that  $\mathbf{J} \cdot \mathbf{E}$  is negative in the depletion region of a pn junction, yet  $\rho J^2$  should always remain positive. (Notice we stated earlier that ohmic conduction was assumed, but that condition does not hold in the depletion region). Thus we are applying an equation in a region where it does not hold. The resolution of this was given by Domenicali [7] for the case of a single carrier;

$$\rho \mathbf{J} \cdot \mathbf{J} = \{[(1/e)(\partial \mu / \partial T) + (1/T)\Pi] \cdot \nabla T\} \cdot \mathbf{J} + \mathbf{J} \cdot \mathbf{E} \quad (6)$$

Here  $\mu$  is the chemical potential; and  $e$  is the magnitude of the electron charge. Observe the Joule heat is only equal to  $\mathbf{J} \cdot \mathbf{E}$  when  $\nabla T = 0$ .

Another term may be added to the right side of Eq. (1) along with Joule heat and Thomson heat; namely the heat generated or absorbed by carrier recombination or generation. This term may be written as  $R E_G$ , ( $R$  is the recombination rate), which is easy to interpret; each recombination releases energy equal to the band-gap; the units are  $\text{W}/\text{cm}^3$ . With this introduction we see we must develop an equation similar to Eq. (5) where all of the correct contributions to general  $\mathbf{q}$  and the source term (right hand side) in Eq. (1) are included. That is we assume the basic 'lattice' conduction term will always be present, and it may be separated from the remaining thermoelectric effects in the equation. Then all of the heat transport mechanisms and all of the heat generation mechanisms will be conveniently lumped into the final  $H$ .

When both electrons and holes are present in a region of a semiconductor device, an expression for  $H$  may be developed from the equations in [3] (a thermoelectric approach). We start with the

fundamental equations in the textbook; they are (1.11.5a, 5b, and 5c)

$$\mathbf{J}_s = -(L_{SS}/T) \nabla T + (L_{Sn}/T) \nabla (\zeta_n/e) - (L_{Sp}/T) \nabla (\zeta_p/e) \quad (7a)$$

$$\mathbf{J}_- = -(L_{nS}/T) \nabla T + (L_{nn}^{(S)}/T) \nabla (\zeta_n/e) - (L_{np}^{(S)}/T) \nabla (\zeta_p/e) \quad (7b)$$

$$\mathbf{J}_+ = -(L_{pS}/T) \nabla T + (L_{pn}^{(S)}/T) \nabla (\zeta_n/e) - (L_{pp}^{(S)}/T) \nabla (\zeta_p/e) \quad (7c)$$

Here  $\mathbf{J}_s$ ,  $\mathbf{J}_-$ ,  $\mathbf{J}_+$  are the entropy, electron, and hole current densities. The terms  $\zeta_n$  and  $\zeta_p$  are the electrochemical potentials for electrons and holes, respectively. The coefficients may be related to the electrical conductivities, Seebeck coefficients, and thermal conductivities; which may be found in Chapters 1 and 3. After identification of the coefficients, the above becomes

$$\mathbf{J}_s = -[(\kappa_L + \kappa'_n + \kappa'_p)/T] \nabla T + \sigma_n \alpha_n \nabla (\zeta_n/e) - \sigma_p \alpha_p \nabla (\zeta_p/e) \quad (8a)$$

$$\mathbf{J}_- = -\sigma_n \alpha_n \nabla T + \sigma_n \nabla (\zeta_n/e) - \sigma_{np} \nabla (\zeta_p/e) \quad (8b)$$

$$\mathbf{J}_+ = -\sigma_p \alpha_p \nabla T + \sigma_{pn} \nabla (\zeta_n/e) - \sigma_p \nabla (\zeta_p/e) \quad (8c)$$

where we have assumed that the coefficient of  $\nabla T$  in the entropy current for the special case when  $\zeta = \zeta_n = -\zeta_p$ , that is for equilibrium, is also valid not too far from equilibrium where  $\zeta_n$  and  $\zeta_p$  are unconstrained. We could use Eq. (1.15.18) of [3] ( $T(\sigma_n \sigma_p / \sigma)(\alpha_n - \alpha_p)^2$ ), in the coefficient of  $\nabla T$  in Eq. (8a), but we neglect it for now. Thus we are assuming near equilibrium conditions where the electrons, holes, and lattice are nearly at the same thermodynamic temperature.

The parameters  $\sigma_{np} = \sigma_{pn}$  are the 'cross-conductivities' that reflect carrier-carrier scattering. The electrochemical potentials may be found from equations in the text; and they are:

$$\zeta_n = kT \cdot \ln(n/N_C) + E_C \quad (9a)$$

$$\zeta_p = kT \cdot \ln(p/N_V) + q\chi + q\psi + E_G \quad (9b)$$

where  $E_C = -q\chi - q\psi$ , as given by Marshak [8]. Here  $q\chi$ ,  $q\psi$ , and  $E_G$  are the electron affinity, electrostatic field energy, and the bandgap energy, respectively. These expressions were not given explicitly in [3], but they may be developed from other equations in the book. The 'cross-conductivities' have been covered by Mnatsakanov [9], and we neglect them here for simplicity. The term  $(\kappa_L + \kappa'_n + \kappa'_p)$  indicates the thermal conductivity due to the lattice, electrons, and holes, respectively. In semiconductors the lattice carries about 95% of the heat, so we neglect  $\kappa'_n$ ,  $\kappa'_p$  for now. Essentially we will treat  $\kappa$  as a variable that depends on the doping and temperature, which may be found in the literature for a given semiconductor. For simplicity we will treat it as a constant when possible. Observe that the electrochemical expressions given cause  $\mathbf{J}_-$  and  $\mathbf{J}_+$  to reduce to the standard forms found in all textbooks; i.e., the sums of drift and diffusion components (when the carrier-carrier scattering and thermal gradients are assumed to be zero).

It is shown [10–12] and elsewhere, that  $\zeta_n = E_F$  (the electrochemical potential is equal to the Fermi level). Using an energy band diagram from Heikes [4], Marshak [8], or Wurfel [13], Fig. 1 shows the relationships between some of the variables in the previous equations.

Observe the subscripts on  $E$ . Both energy differences are called "Fermi levels" referenced to either vacuum or the conduction band edge.

## 2. Thermoelectric development of $H$

The development of  $H$  for the case when electrons and holes exist simultaneously starts with the definition [Eq. (1.10.3)]

$$\mathbf{T} \mathbf{J}_S = \mathbf{J}_E + \mathbf{J}_- (\zeta_n/e) - \mathbf{J}_+ (\zeta_p/e) \quad (10)$$

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