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THE STRUCTURE OF CONSTITUTIVE EQUATIONS FOR SEMICONDUCTOR DEVICES

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ABSTRACT

The fundamental equations that describe carrier transport in semiconductor materials are developed using the methods of continuum mixture theory and Maxwell's equations for electrodynamics. There are five basic equations that govern the behavior of current flux, electrostatic potential, electrons, and holes. The behavior of the electrical chemical potentials are introduced and their relation to the current flux is discussed.

INTRODUCTION

Semiconductor device modeling has a history that dates to about twenty years ago. The literature is extensive and exhaustive, but fortunately several excellent references have been published that contain bibliographies of pertinent literature. A volume, edited by Antognetti, Antoniadis, Dutton and Oldham [1], is a compilation of several survey papers and covers the spectrum of Metal On Silicon - Very Large Scale Integration (MOS-VLSI) modeling. The text by Selberherr [2] is a more in-depth treatment for modeling a basic semiconductor device.

In this paper we shall dwell, primarily, on the derivation of the "fundamental" semiconductor equations. Since our purpose is to offer a derivation based upon continuum thermodynamics, the reader interested in traditional solid-state physics approach should consult Selberherr [2], or Schutz and Potzl [3]. It is noteworthy that the derivation of the so-called fundamental equations of semiconductor devices is credited to Van Roosbroeck [4] in 1950. The equations consist of the Poisson equation, which is essentially the Maxwell equation that relates the divergence of the electric displacement to the electric charge density. There are equations for the continuity of current, one for electrons, and one for holes, which can be derived from Maxwell's equations [2]. Finally, there are the constitutive equations for electron and hole flux.

In what follows, we shall arrive at similar results using ideas borrowed from the continuum theory of mixtures combined with Maxwell's equations.

FUNDAMENTAL SEMICONDUCTOR EQUATIONS I

In this section we develop the semiconductor equations. Certain balance equations are written; in particular, the conservation of charge for electrons, the conservation of charge for holes, and the conservation of energy. It has been demonstrated by Demiray and Eringen [5], also see deGroot and Mazur [6], that the equations of conservation of mass can be interpreted to be identical to the equations for conservation of charge for a mixture where the mobile constituents are electrons and holes. It follows that we assume a priori that mass is conserved for the base semiconductor material.

Our primary sources of reference are the original work of Truesdell [7, 8]; as an aid in organizing the theory, Gurtin [9], Gurtin and Vargas [10], and Serrin [11]; and for a general treatment of continuum electrodynamics, Eringen [12].

The charge mixture is limited to two mobile constituents, electrons, and holes. Following the basic concepts of mixture theory [7, 11, 13], let the charges and their velocities be defined in terms of a mean velocity, v_k ,

$$q v_k = q_n v_{nk} + q_p v_{pk} \quad (1)$$

where

$$q = q_n + q_p \quad (2)$$

and

q_n = charge of the electrons

q_p = charge of the holes

v_{nk}, v_{pk} = velocity of electrons and holes, respectively.

Define a relative current density

$$j_{ak} = q_a (v_{ak} - v_k) ; a = n, p \quad (3)$$

The balance of charge for the ath constituent is

$$\dot{q}_a + q_a v_{k,k} = R_a - j_{ak,k} \quad (4)$$

where R_a is the carrier generation/recombination and $(\dot{\cdot})$ represents the material derivative, $\partial/\partial t + v_k (\cdot)_{,k}$.

Summing on a gives the balance of charge for the mixture as

$$\dot{q} + q v_{k,k} = R \quad (5)$$

and it follows that

$$\Sigma j_{ak} = 0 \quad (6)$$

The balance of energy for the mixture is written as [10, 11, 12]

$$\rho \dot{e} + (h_k + k_k)_{,k} - \rho E_{ak} \dot{P}_{ak} - R_a \nu_a - \rho r = 0 \quad (7)$$

where

ρ = density

e = internal energy

- h_k = heat flux
- k_k = diffusive work term
- E_{ak} = partial electric field
- P_{ak} = partial polarization
- r = external heat supply
- μ_a = electron or hole chemical potential

Following [10] the entropy inequality is proposed as

$$\rho \dot{\eta} \theta + h_{k,k} - h_k \theta_{,k} / \theta - \rho r \geq 0 \quad (8)$$

here

- η = entropy
- θ = temperature ($\theta > 0$)

A free energy function is assumed as [12]

$$F = e - \theta \eta - P_{ak} E_{ak} \quad (9)$$

and it follows that

$$\dot{F} = \dot{e} - \theta \dot{\eta} - \eta \dot{\theta} - P_{ak} \dot{E}_{ak} - E_{ak} \dot{P}_{ak} \quad (10)$$

Equations (7), (8), and (10) are combined to give the general inequality

$$\rho (\dot{F} + \eta \dot{\theta} + P_{ak} \dot{E}_{ak}) + h_k \theta_{,k} / \theta - R_a \mu_a \geq 0 \quad (11)$$

The construction of a constitutive theory is based upon an assumed function, H , that contains the primitive variables that describe the physical problem. The simplest function that yields a constitutive structure similar to the fundamental semiconductor equations is as follows. Let

$$H = H(q_a, \theta, E_{ak}, q_{a,k}) \quad (12)$$

In this instance we have assumed an isothermal situation. We assume the constraints imposed by equipresence are valid and write the following functional relations.

$$F = F(H)$$

$$\begin{aligned}
e &= e(H) \\
\eta &= \eta(H) \\
j_{ak} &= j_{ak}(H) \\
h_k &= h_k(H) \\
k_k &= k_k(H) \\
P_{ak} &= P_{ak}(H) \\
\mu_a &= \mu_a(H)
\end{aligned} \tag{13}$$

Equation (13)₁ leads to

$$\dot{F} = \dot{q}_a \partial F / \partial q_a + \dot{\theta} \partial F / \partial \theta + \dot{E}_{ak} \partial F / \partial E_{ak} + \dot{q}_{ak} \partial F / \partial q_{ak} \tag{14}$$

Equations (4) and (14) are substituted into (11) to give still another form of the inequality

$$\begin{aligned}
\rho \dot{\theta} (\eta + \partial F / \partial \theta) + \rho \dot{E}_{ak} (P_{ak} + \partial F / \partial E_{ak}) - \dot{q}_a (\mu_a - \partial F / \partial q_a) + h_k \dot{\theta}_{,k} / \theta \\
> (k_k - \mu_a j_{ak})_{,k} + \mu_{ak} j_{ak} - q_a \mu_a v_{ak,k} \geq 0
\end{aligned} \tag{15}$$

The theory must formally satisfy the following

$$\begin{aligned}
F &= F(q_a, \theta, E_{ak}) \\
\eta &= -\partial F / \partial \theta \\
P_{ak} &= -\partial F / \partial E_{ak} \\
\mu_a &= \partial F / \partial q_a \\
k_k &= \mu_a j_{ak} \\
h_k &= 0 \\
\partial F / \partial q_{a,k} &= 0 \\
\mu_{a,k} j_{ak} - q_a \mu_a v_{ak,k} &\geq 0
\end{aligned} \tag{16}$$

Equation (16)₁ implies a specific form for the free energy. Equation (16)₅ defines the diffusive work term that was introduced in the energy balance equation.

Let F be expanded in a power series in terms of q_n, q_p, E_{nk}, E_{pk} and

θ and neglect terms higher than the second order. Following Eringen [12] we arrive at the following expression for the free energy.

$$F = f_a q_a^2/2 + f_\theta \theta^2/2 + f_{akl} E_{ak} E_{al}/2 - f_{\alpha\beta} q_\alpha q_\beta - f_{\theta a} \theta q_a \\ - f_{\alpha\beta k} E_{\alpha k} q_\beta - f_{ak} E_{ak} \theta - f_{\alpha\beta kl} E_{\alpha k} E_{\beta l} \quad (\alpha \neq \beta) \quad (17)$$

The relative diffusive flux, j_{ak} , is of practical interest and we assume the simplest possible linear constitutive equation that is allowed by equation (13).

$$j_{ak} = M_{a\beta} q_{\beta,k} + N_{a\beta} E_{\beta k} \quad (\text{sum on } \beta) \quad (18)$$

where $M_{a\beta}$ and $N_{a\beta}$ may be functions of the primitive variables. Note, that to within a first order approximation E_{ak} is the electric field, E_k [2]. Neglecting cross-coupling in equation (18) gives

$$j_{nk} = M_n q_{n,k} + N_n E_k \quad (19)$$

$$j_{pk} = M_p q_{p,k} + N_p E_k \quad (20)$$

where N_n is a function of n and N_p is a function of p . Assume that spacial and material time derivatives can be reduced to the same coordinate system and write (4), taking into account (6),

$$\partial q_n / \partial t = j_{nk,k} - R \quad (21)$$

$$\partial q_p / \partial t = -j_{pk,k} - R \quad (22)$$

The fifth fundamental equation is the Poisson equation that relates the electric field to the electrostatic potential,

$$E_k = -\psi_{,k} \quad (23)$$

and [2]

$$\psi_{,kk} = (q_n - q_p + C)/\epsilon \quad (24)$$

where C is an external source and ϵ is the dielectric constant.

FUNDAMENTAL SEMICONDUCTOR EQUATIONS II

We are motivated by the discussion in [2] and by the typical results reported by such researchers as Lundstrom, Schwartz and Gray [14] and Polisky and Rimshans [15] to assume that the partial electric field of equation (12) exists along with its gradient. We replace (12) with

$$H = H(q_a, \theta, E_{ak}, q_{a,k}, E_{ak,k}) \quad (25)$$

and add to equation (16) $\partial F / \partial E_{ak,k} = 0$. Equation (17) remains unchanged, but we can modify equation (18). Assume that j_{ak} , the relative current density, is driven by gradients of the primitive variables. Therefore,

$$j_{a,k} = M_{a\beta} q_{\beta,k} + L_{a\beta k} E_{\beta i,i} \quad (26)$$

where the notation allows for possible cross-coupling. However, neglecting cross-coupling gives the following for the current.

$$j_{nk} = M_n q_{n,k} + L_{nk} E_{ni,i} \quad (27)$$

$$j_{pk} = M_p q_{p,k} + L_{pk} E_{pi,i} \quad (28)$$

It follows from equation (17), neglecting cross-coupling and temperature effects,

$$\mu_n = \partial F / \partial q_n = f_n q_n - f_{nk} E_{ni} \delta_{ik} \quad (29)$$

$$\mu_p = \partial F / \partial q_p = f_p q_p - f_{pk} E_{pi} \delta_{ik} \quad (30)$$

The familiar relation between flux and chemical potential, namely, that the flux is proportional to the gradient of the chemical potential, now exists when equations (27) - (30) are compared. The semiconductor equations (21), (22), and (24) remain unchanged.

The equations that have been presented illustrate that the formality that exists within the framework of continuum thermodynamics may give additional insight for the problems that arise in modeling semiconductor devices.

TEMPERATURE EFFECTS

We have, in this brief outline, avoided introducing temperature effects. The first step would be to include the temperature gradient in the list of primitive variables. We visualize that the heat flux, as well as the temperature gradient, would appear in the general statement of entropy inequality. The gradients of temperature would then be included in the general constitutive equations for current, equations (27) and (28). In addition, the electrical chemical potentials would be functions of

temperature. The heat flux would then be written as a function of gradients of electrons, holes, electric field, and temperature. Hence, a fairly complete theory is visualized. We have not found such a complete theory in the literature. A paper by Gaur and Navon [16] is representative of the inclusion of temperature effects for studying semiconductors.

One last remark is in order; the energy balance equation, equation (7), can be recast in a more usable form. Substitute equations (4) and (10) into (7). Recall that equation (16₆) requires that $q_k = 0$ and the energy balance becomes

$$\rho \dot{\theta}_n + \mu_{n,k} j_{nk} + \mu_{p,k} j_{pk} - \rho r = 0 \quad (31)$$

Equation (31) is a more useful form of the energy equation for numerical computation.

CONCLUSIONS

The fundamental semiconductor equations have been discussed from the viewpoint of continuum thermodynamics. Constitutive equations for current density were developed and electrical chemical potentials were introduced. The effects of temperature gradients and strain gradients were not included, but are the topic of future work. Finally, the authors offer an apology to the solid-state physics community for not adhering to accepted nomenclature.

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