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Mechanisms of the thermal electromotive force, heating and cooling in semiconductor structures

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ABSTRACT

A comprehensive study of the mechanisms of the thermal electromotive force, heating and cooling originated by a temperature gradient and an electric current in semiconductor devices is reported. The Seebeck, Peltier, Joule and Thomson phenomena are studied self-consistently under the approximation of weak electric current and temperature gradient. Analytical calculations show that the contributions of each effect to the temperature distribution are commensurable. A new formulation and interpretation of the Thomson effect are given. Additionally, attention is paid to some questions of nonequilibrium thermodynamics of thermoelectric and electrothermic phenomena, that demand some clarification.

1. Introduction

The problem of heating/cooling is currently of a paramount importance for the progress of semiconductor devices and circuits since the heat dissipation imposes severe limits to the increasing integration density of elements of modern micro-/nano-electronic circuits [1]. Additionally, there is a growing market for thermoelectric cooling applications [2].

Three well-known physical phenomena are considered to be responsible for changes in temperature of a semiconductor structure under the action of an electric current, namely, Peltier, Joule and Thomson effects [3]. Nevertheless, from classic textbooks [4,5] to the most recent publications [3,6] there has been a systematic lack of comprehensive mathematical formulation aimed to unravel the heating/cooling problem as a whole. Instead, each effect has normally been studied under special conditions in order to exclude the influence of the two others. Since the three effects have been studied separately, it is somewhat difficult to accurately calculate the temperature distribution in a real device operating under practical conditions, since none of these special conditions take place. Because in the case of biased devices the final temperature distribution results from a combination of all the three mechanisms, a thorough understanding of their simultaneous action is crucially important.

Recently published results [7] have shown that the change in temperature associated to the Peltier effect is not related to the presence of heat sources and sinks. The Peltier effect may be written as: $(\Pi_1 - \Pi_2)\vec{j}$, $\vec{j}$ being the electric current density and Π the Peltier coefficient (the subscripts are for two media 1 and 2), Π may be written as $\Pi = \alpha T$ (α being the Seebeck coefficient and T is temperature). In contrast, this temperature change is related to the appearance of the diffusion heat flux, $\vec{q}_{diff} = -\kappa\nabla T$, which, following the Le Châtelier–Braun principle [8], compensates the change in the drift component of the heat flux ($\vec{q}_{dr} = \Pi\vec{j}$), κ being the thermal conductivity.

The Thomson effect is commonly regarded as a heat source/sink $[-T(d\alpha/dT)\vec{j}\nabla T]$, which should be added to the Joule heating [3–6]. Nevertheless, in a recently published work [9], it was clearly shown that this formulation of the Thomson effect is essentially erroneous, since, if consistently formulated, this effect may exist even if $d\alpha/dT = 0$ and, moreover, the expression $-T(d\alpha/dT)\vec{j}\nabla T$ is not a heat source/sink. The last point is very important since the Thomson effect is often neglected adducing that because its proportionality to $d\alpha/dT$ it should vanish when the kinetic coefficients do not depend on the temperature. This is an approximation widely used in the literature. In strong contrast to it, in recently published

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Nomenclature

Roman symbols

e	absolute value of the electron charge (C)
E	thermal electromotive force (EMF) in the circuit (V)
$\vec{j}$	electric current density (A m^{-2})
l, L	length (m)
$\vec{q}$	flux of kinetic energy (J m^{-2})
$\vec{q}_{diff}$	diffusion heat flux (W m^{-2})
$\vec{q}_{dr}$	drift heat flux (W m^{-2})
T	temperature (K)
u_i	voltage's drops (V)
$\vec{w}$	energy flux (W m^{-2})

Greek symbols

α	Seebeck coefficient (V/K)
α_s	surface Seebeck coefficient (V/K)
$<\varepsilon>$	average value of the electrons kinetic energy (J)
κ	thermal conductivity (W/K)
μ	chemical potential (V)
Π	Peltier's coefficient (V)
σ	electrical conductivity (Ω m^{-1})
σ_{ext}	electrical conductivity of the external circuit (Ω m^{-1})
σ_s	surface electrical conductivity (Ω m^{-2})
ν	heat source density (W m^{-3})
$\tilde{\varphi}$	electrochemical potential (V)
$\tilde{\varphi}_{ext}$	electrochemical potential of the external circuit (V)
φ	electric potential (V)

results [7,9] it was shown that the Thomson effect exists even if the kinetic coefficients are temperature-independent and its magnitude is similar to the one of the Joule effect (see below).

Finally, it should be noted that, as stated above, the study of the three effects as completely separate phenomena [3–6] can lead to serious errors. For instance, let us consider a sample under an electric current in conditions such that the Peltier effect takes place; this will create a temperature gradient, consequently, the Thomson effect will naturally take place in a second-order approximation with respect to electrical current (i.e. the Thomson and the Joule effects will be of the same order, of magnitude) and it cannot be ignored. Some aspects of this problem were discussed in Refs. [9–11].

If instead of an electrical current a gradient of temperature is present, the Seebeck effect will setup a current in the circuit and all the three effects will simultaneously take place as above stated.

2. Energy, heat and charge fluxes in thermoelectric and electrothermic phenomena

Commonly, thermoelectric effects are described in terms of the Seebeck, Peltier and Thomson effects mentioned above. This terminology has developed historically and in some cases it is not properly related to the essence of the phenomena. Even though, the attribute used in the name of a phenomenon must unambiguously reflect its cause and effect errors commonly arise. In the thermoelectric effect an electric current is generated by a temperature difference that creates a heat flux in a thermoelectric circuit and, subsequently, a flux of charge carriers. For this reason the Seebeck effect undoubtedly belongs to the category of *thermoelectric* phenomena.

On the contrary, in the Peltier effect an external source of electric current is the cause that induces, in a non-uniform closed circuit, thermal diffusion heat fluxes and, as a consequence, temperature distributions that may result in a temperature drop as compared to a reference equilibrium value. In this case, it is more correct to classify the Peltier as *electrothermal* [12].

Similarly, the heating of charge carriers in an external electric field (Joule effect) must be regarded as a thermoelectric effect if the electric current is generated by the thermal electromotive force (thermal EMF). On the contrary, if the electric current has an external source, this effect should be classified within the electrothermal ones. In the first case the effect is quadratic in terms of the temperature difference between the heater and the cooler, while in the second case the effect is quadratic in terms of the electric current.

Within this classification the Thomson effect is also defined by the process studied: generating thermal EMF or cooling. In the first case it is an effect of thermoelectric nature and has a quadratic dependence of the temperature difference between the heater and the cooler as the electric current is proportional to it. Thus, the Joule thermoelectric effect and the Thomson thermoelectric effect are of the same order in terms of the temperature difference ΔT.

In the Peltier effect the gradient of temperature appears as a consequence of the electric current in a non-uniform environment. It is clear that in this case the Thomson effect is electrothermal. In this case it is quadratic in the electric current as well as the Joule electrothermal effect [9].

One can consider a closed electric circuit in which *a priori* there are both a temperature gradient created by a thermal contact with external thermostats and an electric current created by an external source. Usually in literature Thomson effect was studied under this condition. In this case it is impossible to classify neither the Joule effect nor the Thomson effect as thermoelectric or electrothermal phenomena. However, such circuits are of little interest for practical applications and in the present paper we propose the study in very different conditions.

Both thermoelectric and electrothermal effects take place in closed circuits where energy, heat and charge flow simultaneously. In spite of the fact that the definitions of these fluxes have been well known for a long time, in a number of references they are given by different expressions. This is a direct consequence of the fact that in any expression involving fluxes (energy, kinetic energy, and/or heat energy charge flux) for forces are gradients of temperature and of electrochemical potential; the latter being dependent also on the temperature gradient.

For example, in Ref. [5] the energy flux is written as:

$$\vec{w} = -\kappa\nabla T + (\Pi + \tilde{\varphi})\vec{j}, \tag{1a}$$

where $\tilde{\varphi} = \varphi + (\mu/e)$ is the electrochemical potential, φ and μ are the electric and chemical potentials, respectively, e is a carrier charge (for electrons it is negative); whereas in Ref. [13] the same flux is defined as:

$$\vec{w} = -\kappa\nabla T + \left(\Pi + \frac{\mu}{e}\right)\vec{j}. \tag{1b}$$

The heat flux $\vec{q}$ in Ref. [14] is written as:

$$\vec{q} = -\kappa\nabla T + \Pi\vec{j}. \tag{2a}$$