

Thermodynamic Treatment of Mechanical Stress Gradients in Coupled Electro-Thermo-Mechanical Systems

Koorosh Aflatooni, Richard Hornsey and Arokia Nathan

Electrical and Computer Engineering, University of Waterloo
Waterloo, Ontario N2L 3G1, Canada

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Using the principles of irreversible thermodynamics and, notably, Onsager's theorem, we provide a complete and consistent description of electrical, thermal and mechanical interactions and their mutual coupling for accurate modeling of mixed signal microsystems. We reproduce earlier predictions based on the microscopic transport theory which have demonstrated how a mechanical stress gradient could result in the flow of electrical or heat currents. In addition, it is now shown that a gradient in temperature, electrochemical potential or mechanical stress can lead to a so-called "strain flux." A physical interpretation of the strain flux and its constituent terms is presented along with its relation to the well-known thermoelasticity equation.

1. Introduction

We are currently witnessing rapid proliferation of increasingly complex microsystems (*e.g.* MEMS) for sensor and actuator applications. These microsystems are inherently three-dimensional structures with physical dimensions ranging from micrometers to millimeters and rely on integrated circuit microfabrication techniques coupled with application-specific thin-film deposition and micromachining technologies. Owing to their small physical dimensions, the electrical, thermal or mechanical conditions may become relatively extreme, so the mutual coupling of effects is significant. Thus, effects traditionally considered to be second order in macroscopic systems may no longer be ignored. In view

of the large number of design parameters and the complexity of various interactions, computer simulation tools are becoming an integral part of the design process. Hence, a complete and consistent formulation which accounts for the coupling of different energy fields is necessary to accurately describe the behavior of the microsystem.

Nonuniform stresses or stress gradients typically arise in microstructures, for example, at the vicinity of the clamped end of a displaced cantilever beam or from differences in thermal expansion coefficients between constituents of a multilayer sandwich. It has been previously shown, using the microscopic transport theory, that a stress gradient can lead to the flow of electrical⁽¹⁾ and heat⁽²⁾ currents. In the former case, the current flow was found to be due to the combined stress-dependencies of the semiconductor bandgap and the electronic density of states. The heat flow is the result of phonon diffusion that arises due to a stress-induced change in the phonon distribution. In this work, we have developed, using principles of irreversible thermodynamics, a system of phenomenological equations that account for the interactions of a stress gradient with electrical and heat transport. Here, we not only derive generalized expressions for the electrical and heat fluxes in terms of the various driving forces, including mechanical stress gradient, but we obtain an additional equation that stems from these driving forces which constitutes a "strain flux."

2. Thermodynamic Treatment

Irreversible thermodynamics combines equilibrium thermostatics with time reversal symmetry in order to analyze the rates at which physical processes occur. Integral to this approach is the Onsager reciprocity theorem⁽³⁾ which states that, if a physical system consists of a number of driving forces and resultant fluxes, there will be symmetry between the linear relationship connecting the j^{th} driving force and the k^{th} flux and between that connecting the k^{th} force and the j^{th} flux. This allows a set of relations to be derived which expresses each flux in terms of the sum of the components arising from each driving force, thereby providing information on the nature of the cross-coupling terms. The generalized forms of these driving forces are referred to as "affinities," and the fluxes represent the rates of change of extensive parameters of the system. In these nonequilibrium situations, it is assumed that the dependence of a parameter upon the local intensive parameters (such as temperature, pressure or electrochemical potential) is the same as that in equilibrium.

We introduce our analysis by first revisiting the more familiar coupled equation system that describes thermoelectric effects. We then extend the system to include the effects of a mechanical stress gradient and follow this with a discussion on the physical interpretation of resulting expressions.

We follow the approach performed by Callen.⁽⁴⁾ The thermodynamic treatment is simplified if a flux, J_k , of a particular extensive parameter at a given time is assumed to depend only on the instantaneous values of the affinities, f , and intensive parameters, F . This can be expressed as

$$J_k = J_k(f_0, f_1, \dots; F_0, F_1, \dots). \quad (1)$$

Thus, while a particular flux depends mainly on its associated affinity, it will also be affected by other affinities. Since we know that the flux must be zero in the absence of any affinities, the constant term in the Taylor expansion of eq. (1) will also equal zero. Therefore, eq. (1) can be re-written as

$$J_k = \sum_j L_{jk} f_j + \frac{1}{2!} \sum_i \sum_j L_{ijk} f_i f_j + \dots, \quad (2)$$

where $L_{jk} = (\partial J_k / \partial f_j)_0$ are known as kinetic coefficients and are simply functions of the intensive parameters. Moreover, the system can be further constrained to be both resistive and linear, in which case the higher order terms in eq. (2) can be neglected, giving

$$J_k = \sum_j L_{jk} f_j, \quad (3)$$

or in terms of an entropy current density, \mathbf{J}_s , which in vector form reads⁽⁴⁾

$$\mathbf{J}_s = \sum_k F_k \mathbf{J}_k, \quad (4)$$

where \mathbf{J}_k denotes a flux density. Equation (4) states that the entropy flux density is equal to the sum of the flux density of each extensive parameter multiplied by its associated intensive parameter. It is assumed that the rate of production of entropy (\dot{s}) at any point is equal to the rate of increase of entropy ($\partial s / \partial t$) at that point plus the flux of entropy leaving that point. Thus, we find

$$\dot{s} = \frac{\partial s}{\partial t} + \nabla \cdot \mathbf{J}_s, \quad (5)$$

which can be simplified to give

$$\dot{s} = \sum_k \nabla F_k \cdot \mathbf{J}_k. \quad (6)$$

Therefore, the local rate of production of entropy is given by the sum of the products of each flux with its associated affinity which, for continuous systems, is defined as the local gradient of the entropy-representation intensive parameter, F_k . It is this entropy change that determines the irreversibility of the process.

In the specific example of thermoelectric effects, the entropy relation is

$$Tds = du - \sum_k \mu_k dn_k, \quad (7)$$

where ds denotes the change in entropy per unit volume, u represents the local energy density, μ_k is the electrochemical potential per particle and n_k is the number of particles per unit volume. The second term on the right-hand side of eq. (7) represents the work performed on the system. Equation (7) can be re-written using eq. (4) to give an expression for \mathbf{J}_S ,

$$\mathbf{J}_S = \frac{1}{T} \mathbf{J}_U - \frac{\mu}{T} \mathbf{J}_N, \quad (8)$$

where \mathbf{J}_U and \mathbf{J}_N are the heat and electric flux densities, respectively. The terms $(1/T)$ and $-(\mu/T)$ represent the appropriate forms of the intensive parameter, F_k , in eq. (4). By an analogy with eq. (6), the expression for the rate of production of entropy is therefore

$$\dot{s} = \nabla \cdot \frac{1}{T} \mathbf{J}_U - \nabla \cdot \frac{\mu}{T} \mathbf{J}_N. \quad (9)$$

This expression allows us to associate the affinity, $\nabla(1/T)$, with the heat flux density, \mathbf{J}_U , and the affinity, $\nabla(\mu/T)$, with the electrical flux density, \mathbf{J}_N . The dynamical equations for the individual electrical and heat flux densities can be written as

$$-\mathbf{J}_N = L'_{11} \nabla \frac{\mu}{T} + L'_{12} \nabla \frac{1}{T} \quad (10)$$

$$\mathbf{J}_U = L'_{21} \nabla \frac{\mu}{T} + L'_{22} \nabla \frac{1}{T}. \quad (11)$$

In this form, the Onsager theorem⁽³⁾ can be used to relate the cross-coupling terms L'_{12} with L'_{21} . For example, $L'_{12} = L'_{21}$ or in the presence of a magnetic field, \mathbf{B} , $L'_{12}(\mathbf{B}) = L'_{21}(-\mathbf{B})$. Here, we used the "prime" notation to distinguish the specific kinetic coefficients from the general case given in eq. (2).

3. Inclusion of Stress Gradient

To include stress gradients, an extra term must be added to the entropy relation, eq. (7), to account for the work performed on the system by the stress. This work is simply the applied force times the distance over which it acts, so the work performed per unit volume is equal to $\chi \varepsilon$, where χ is the stress and ε is the strain. The entropy relation modified from eq. (7) is thus

$$ds = \frac{du}{T} - \sum_k \left(\frac{\mu_k}{T} \right) dn_k - \sum_{ij} \frac{\chi_{ij}}{T} d\varepsilon_{ij}. \quad (12)$$

Not only does the inclusion of the stress component add extra terms to the dynamic equations, it also introduces a third equation. Following the same arguments employed in the above thermoelectric case, the dynamic equations are found to be

$$-\mathbf{J}_N = L'_{11} \nabla \frac{\mu}{T} + L'_{12} \nabla \frac{1}{T} + L'_{13} \nabla \frac{\tilde{\chi}}{T}, \quad (13)$$

$$\mathbf{J}_U = L'_{21} \nabla \frac{\mu}{T} + L'_{22} \nabla \frac{1}{T} + L'_{23} \nabla \frac{\tilde{\chi}}{T}, \quad (14)$$

$$-\mathbf{J}_\varepsilon = L'_{31} \nabla \frac{\mu}{T} + L'_{32} \nabla \frac{1}{T} + L'_{33} \nabla \frac{\tilde{\chi}}{T}, \quad (15)$$

where \mathbf{J}_ε denotes the density of "strain flux," $\tilde{\chi}$ is the stress tensor and $\nabla \tilde{\chi} = \sum_{ij} \nabla \chi_{ij}$.

The Onsager theorem can still be used to relate the individual kinetic coefficients which are dependent on the intensive parameters (T , μ , and χ). Note that due to stress-induced material anisotropies, these kinetic coefficients become tensors. We now proceed to discuss the physical interpretation of the additional terms in eqs. (13) and (14) and the additional equation, eq. (15).

4. Interpretation

Some limitations to the thermodynamic approach are apparent. First, information is only available concerning the qualitative relationships between effects, not the magnitudes. Second, the above derivations are for ideal materials and, moreover, they do not account for external restoring forces that might be present in practical systems. Third, the analysis does not specify which material is being considered, so the magnitude of each effect will vary from material to material.

The three terms on the right-hand side of eqs. (13) to (15) represent the influence of gradients in electrochemical potential, temperature and stress on the fluxes in question. For convenience, we consider a homogeneous material. Here, the electrochemical potential, μ , can be reduced to its electrical component; in this case, $\nabla \mu$ describes the electric field in the material.

Equation (13) indicates that the electrical flux density, \mathbf{J}_N , is dependent on the electric field, as would be expected, and on the temperature gradient, $\nabla (1/T)$; the latter represents the Seebeck effect. The third term on the right-hand side of eq. (13) demonstrates that a stress gradient can lead to charge flow. This is a general form of the effect reported by Manku and Nathan⁽¹⁾ whereby stress-induced changes in the bandgap and the electron

density of states can lead to an electrical current. It should be noted that a uniform stress, $\nabla\chi = 0$, has the effect of altering the entire material isotropically, therefore there can be no net flow of charge.

\mathbf{J}_U is strictly the flux density of internal energy, but this term is more usually thought of as a heat flow. Clearly, a temperature gradient, the second term in eq. (14), will lead to a heat flow, while the $\nabla\mu$ term represents the heat flow due to the Peltier effect. The presence of a stress gradient can also lead to heat flux;⁽²⁾ positional differences in the lattice spacing of the material brought about by the stress cause spatial variations in the phonon energy distribution which can act as a "driving force" for heat flow. Again, a uniform stress will cause the same lattice distortions spatially, precluding heat flow by this mechanism.

Before interpretation of the physical processes embodied in eq. (15), the meaning of the "strain flux" must first be established. A strain is essentially a deformation or, alternatively, an expansion or contraction of a material, implying a change in the atomic spacing. Hence, a flux of strain must represent a nonisotropic expansion or contraction, thereby causing a net "flow" or migration of material in a preferred direction. Using this definition for \mathbf{J}_ϵ , it follows that a uniform stress cannot contribute to strain flux, as described by the last term in eq. (15), because it would deform the material isotropically with no net material movement.

The first term on the right-hand side of eq. (15) indicates that the strain flux is linearly dependent on the electric field, $\nabla\mu$. Because of this linear relationship and the dependence of the flux on the polarity of $\nabla\mu$, this effect cannot be caused by the electric-field-induced polarization of initially unpolarized atoms. This so-called dielectrophoresis requires a nonuniform electric field and the force on the atoms is independent of the field direction.⁽⁵⁾ Instead, the $\nabla\mu$ term can be assigned to the piezoelectric effect. Here, the atomic structure of the material is already polarized, leading to the required linear and directional dependence of the mechanical deformation on the applied electric field. In familiar macroscopic examples of the piezoelectric effect, the motion of a mechanical structure ceases when an equilibrium is reached between the piezoelectric force induced by the applied electric field and the restoring force of the material itself. Such equilibration is not described in the present thermodynamic formulation.

The remaining term in eq. (15) describes how a temperature gradient can lead to an anisotropic thermal expansion (or contraction) of the material. This phenomenon is well known in mechanical engineering as the thermoelastic effect.⁽⁶⁾ We now proceed to demonstrate that, in the absence of applied electrochemical or stress gradients, eq. (15) can be reduced to the steady state linear thermoelasticity equation.

First, we assume that extensive parameters, such as the strain, are conserved, in which case we find a continuity relation

$$\nabla \cdot \mathbf{J}_\epsilon = -\frac{\partial \tilde{\epsilon}}{\partial t}, \quad (16)$$

where $\tilde{\epsilon}$ denotes the strain tensor. Taking the divergence of eq. (15) and assuming that there are no gradients of electrochemical potential or stress, we obtain

$$-\nabla \cdot \mathbf{J}_\varepsilon = \nabla \cdot \left[L'_{32} \nabla \left(\frac{1}{T} \right) \right] = L'_{32} \nabla \cdot \nabla \left(\frac{1}{T} \right), \quad (17)$$

where L'_{32} is a constant. Simplifying eq. (17) and neglecting higher order terms (such as $\nabla T \cdot \nabla T$), we find

$$-\nabla \cdot \mathbf{J}_\varepsilon = L'_{32} \nabla^2 T. \quad (18)$$

Making use of eq. (16), we derive the final expression

$$\frac{\partial \tilde{\varepsilon}}{\partial t} = L'_{32} \nabla^2 T. \quad (19)$$

The linear form of the thermoelasticity equation, valid for small changes of temperature, is⁽⁶⁾

$$\kappa \nabla^2 T = C_1 \frac{\partial \tilde{\varepsilon}}{\partial t} - C_2 \frac{\partial T}{\partial t} - \rho_0 R, \quad (20)$$

where κ is the thermal conductivity, $C_{1,2}$ are coefficients, ρ_0 is the mass density and R is the heat produced per unit time and per unit volume. If the rate of change of strain is constant, the resulting spatial temperature differential is also time independent, and hence, $\partial T / \partial t = 0$. We further assume that there is no internal heat production, $R = 0$, therefore, eq.(20) becomes

$$\frac{\partial \tilde{\varepsilon}}{\partial t} = \frac{\kappa}{C_1} \nabla^2 T, \quad (21)$$

which is clearly of the same form as eq. (19). An interesting corollary of eq. (21) is that application of a time-varying compressive strain ($\partial \varepsilon / \partial t$ negative) will heat the material while a tensile strain will cool the material. The latter case is known as the Gough-Joule effect⁽⁶⁾ and the conversion of mechanical deformation into heat, an irreversible process, can lead to thermoelastic damping of vibrations in mechanical structures.⁽⁷⁾

5. Conclusions

In this paper we have developed a system of phenomenological equations that describes the interaction of a mechanical stress gradient with electrical and heat transport. Generalized expressions were developed for the electrical and heat fluxes in terms of, not only the well-known driving forces (*e.g.*, gradient in electrochemical potential and temperature), but also in terms of a mechanical stress gradient. In addition, these driving forces lead to a strain flux. This can be related to the well-known thermoelasticity equation.

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