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TEMPERATURE, HEAT TRANSPORT AND DISLOCATIONS

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ABSTRACT. We examine three basic aspects of the relation between dislocations and heat transport: a) the role of dislocations on thermal conductivity; b) the contribution of dislocations flux to the heat flux, and c) the definition of dislocation temperature in non-equilibrium states.

1. Introduction

Understanding the role of internal variables on heat transport is an interesting topic in materials engineering, in order to achieve the most convenient situations for several applications. This topic has three well-defined aspects: a) how the internal variables modify the thermal conductivity in steady states; b) how the flux of moving internal variables contributes to the heat flux; c) what is the meaning of temperature of the corresponding variables and their relation to heat transport. In particular, in this paper we explore these points in connection to dislocations in solids. Dislocations are described here as internal variables in contrast to the usual variables of the lattice, namely, kinetic and elastic degrees of freedom, respectively related to speed and position of the particles.

In Section 1 we briefly report some observations on the influence of dislocations on thermal conductivity. In Section 2 we consider evolution equations of the heat field and the dislocations field and their mutual couplings. In Section 3 we deal with caloric and entropic temperature of dislocations. In Section 4 we discuss their contributions to the entropy flux.

2. Thermal conductivity and dislocations

First, we consider the simplest situation of heat conduction in a solid lattice with fixed dislocations. In this case, the only (but very important) role of dislocations will be to modify the thermal conductivity because of their scattering of phonons. This is not properly a topic for thermodynamics, but for statistical physics and transport theory, but it is important to underline the main physical features as a practical motivation for the present work. Indeed, this reduction in thermal conductivity hinders the rate of removal of excess heat produced in some laser diodes, microwave power sources, as ultrahigh power switches, thus affecting their respective performances.

The effect of dislocations on thermal conductivity and other transport coefficients (electrical conductivity, Seebeck coefficient) has been well studied from the experimental and theoretical points of view (Kotchetkov *et al.* 2001; Zou *et al.* 2002; Mion *et al.* 2006; Watting and Paul 2011; Ma *et al.* 2013; Ni *et al.* 2014). It is found that the dislocation density ρ_D (total length of dislocation lines per unit volume, which has units of (length)$^{-2}$) has only a minor effect on the thermal conductivity for dislocation densities smaller than a characteristic value dependent on the material and temperature. For higher values, there is a decrease of thermal conductivity. For instance, for Gallium Nitride (GaN) the critical dislocation density is of order of $10^8\ cm^{-2}$. For higher values, the conductivity decreases linearly with the logarithm of the dislocation density (Kotchetkov *et al.* 2001). This is due to phonon-dislocation scattering, which is negligible as compared to phonon-phonon scattering (for small dislocation densities ρ_D) but which becomes dominant for high values of ρ_D.

Furthermore, dislocations reduce electrical conductivity but increase the Seebeck thermoelectric coefficient in some range of dislocation densities $(10^6 cm^{-2} - 10^{10} cm^{-2})$ due to an increase in the entropy of the carriers (Watting and Paul 2011). Thus, for some ranges of dislocation density the efficiency of thermoelectric energy conversion may be raised by dislocations, especially in low-dimensional structures (films, wires or dots). This makes that dislocation engineering is becoming increasingly useful in the optimization of semiconductor devices.

3. Field equations for heat flux and dislocations

In this section, we take the dislocation tensor as a further dynamical variable, instead of taking it as a fixed parameter. Considering a tensorial description gives of course more information than sticking simply to the total dislocation length density (Restuccia and Maruszewski 1995; Mazzeo and Restuccia 2008, 2011; Restuccia 2019). This formulation allows dislocations to evolve, by production, destruction, or motion, and interact with the heat flux.

The evolution of internal variables is described by evolution laws which are different from the so-called constitutive laws, namely the transport equations of heat, mass, charge or momentum. The ensemble of constitutive (transport) laws and the evolution laws of the internal variables describe the evolution of the system. Here, see Restuccia and Maruszewski (1995) and Restuccia (2016, 2019), we assume a crystal with a dislocation field, described by a dislocation tensor a_{ij}, and by its gradient $a_{ij,k}$ (simpler descriptions were proposed years ago based on a scalar variable (Bailey 1963; Ladd and Hoover 1982; Maugin 1999), the dislocation line density, rather than a tensor).

The dislocation tensor describes the local structure of dislocation lines, which form a network of very thin lines disturbing the otherwise perfect periodicity of the crystal lattice. The trace of this tensor is the dislocation density ρ_D introduced in Section 1. In the frame of extended irreversible thermodynamics, thermodynamical models for solids, semiconductors and superlattices with dislocations were derived in Restuccia and Maruszewski (1995), Mazzeo and Restuccia (2008, 2011), Restuccia (2016), Jou and Restuccia (2018a,b), and Restuccia (2019). In this paper, we consider crystals that may also be submitted to an external energy flux $\tilde{\mathbf{q}}$ and then we give a model for our physical problem, where we take into account the effect of this external energy source.

The following fields interact with each other: the thermal field described by the non-equilibrium absolute temperature θ_{neq}, its gradient $\theta_{neq,i}$ and the heat flux q_i; the elastic field described by the total stress tensor σ_{ij} (in general non symmetric) and the small strain tensor ε_{ij}, defined as $\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$, with u_i the components of the displacement vector; the dislocation field described by the dislocation core tensor a_{ij} and its gradient $a_{ij,k}$. The standard Cartesian tensor notation in a rectangular coordinate system is used and the motion of our material system is referred to a current configuration $\mathscr{K}_t$. Then, the independent variables are represented by the set

$$C = \left\{\varepsilon_{ij}, \theta_{neq}, \theta_{neq,i}, a_{ij}, a_{ij,k}, q_i\right\}. \tag{1}$$

All the processes occurring in the considered body are governed by two groups of laws. The first group deals with the classical balance equations, namely:

the continuity equation

$$\dot{\rho} + \rho v_{i,i} = 0, \tag{2}$$

where ρ denotes the mass density, v_i is the velocity of the body point and a superimposed dot denotes the material derivative;

the momentum balance

$$\rho \dot{v}_i - \sigma_{ji,j} - f_i = 0, \tag{3}$$

where σ_{ji} is the symmetric stress tensor and f_i is a given body force;

the internal energy balance

$$\rho \dot{U} - \sigma_{ji} v_{i,j} + q_{i,i} + \tilde{q}_{i,i} = 0, \tag{4}$$

where U is the internal energy density, $\tilde{\mathbf{q}}$ is a given external energy flux. We suppose that $\tilde{\mathbf{q}} = \tilde{\mathbf{q}}_1 + \tilde{\mathbf{q}}_2$, in such a way that $\tilde{\mathbf{q}}_1$ is the source heating the lattice and $\tilde{\mathbf{q}}_2$ is the dislocation source, as it will be illustrated with an example below equations (5).

Dislocations contribute to internal energy by means of their stored energy (Bailey 1963; Ladd and Hoover 1982; Maugin 1999; Restuccia 2016), proportional to the total length, to the shear modulus of the material, and to the square of the modulus of the Burgers vector of the dislocations. Furthermore, there will be the usual kinetic and potential (elastic) contributions of the lattice. When two materials with dislocations are put in thermal contact, they exchange the lattice energy much more efficiently than the dislocation energy. Thus, the temperature of the dislocations, in general, will not be necessarily equal to the kinetic and potential temperatures of the lattice. However, temperature of dislocations is rarely studied. In general, the effects of environment temperature on the dislocations are studied, but not the meaning of temperature for dislocations. This will be considered in Section 4.

The second group of laws deals with *the rate properties of the dislocation core tensor and the heat flux*, respectively

$$\begin{aligned} \dot{a}_{ij} + \mathscr{V}_{ijk,k} - A_{ij}(C) - \tilde{A}_{ij}(\tilde{\mathbf{q}}_2) &= 0, \\ \dot{q}_i - Q_i(C) - \tilde{Q}_i(\tilde{\mathbf{q}}_1) &= 0, \end{aligned} \tag{5}$$

where $\mathscr{V}_{ijk}$ is the dislocation flux tensor, $A_{ij}(C)$ and $\tilde{A}_{ij}(\tilde{\mathbf{q}}_2)$ are the internal and external sources of dislocations, and $Q_i(C)$ and $\tilde{Q}_i(\tilde{\mathbf{q}}_1)$ are the internal and external sources for the

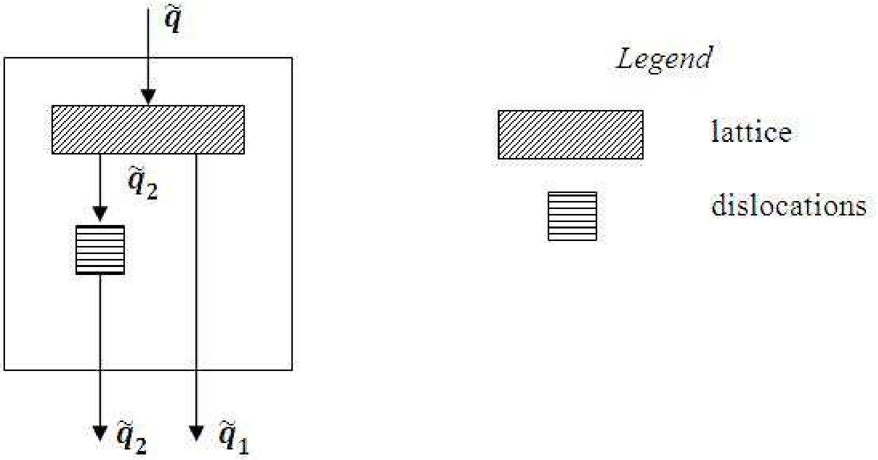

FIGURE 1. A thermodynamic system submitted to an external energy flux $\tilde{\mathbf{q}}$. A part of this flux heats the lattice ($\tilde{\mathbf{q}}_1$) and the other part ($\tilde{\mathbf{q}}_2$) produces some dislocations

heat flux, respectively. For instance, one could have in mind the walls of a fusion nuclear reactor, which are submitted to an intense neutron flux supplied by the nuclear reaction of deuterium and tritium giving He^4 and neutrons. This neutron flux on the walls acts as an energy supply in two different aspects (see Fig.1): a purely thermal flux (it heats the walls) which we denote as $\tilde{\mathbf{q}}_1$, and a supply $\tilde{\mathbf{q}}_2$, that produces defects or dislocations in the walls. In other terms, $\tilde{\mathbf{q}}_2$ could be interpreted as the part of the energy flux whose carriers have enough individual energy to produce some new dislocation. The second effect is unwanted, because it may reduce the mechanical resistance of the wall. In the simplified version presented here, we describe the mechanical effects of the neutrons through a field of induced dislocations.

In the absence of dislocations, the system would be described by a thermal field depending on the non-equilibrium temperature, and by an elastic field described by a local small strain tensor ε_{ij}. Dislocations may be measured by suitable methods (for instance, electronic microscopy), but cannot be controlled - one can try to control the method of crystal growth in order to reduce the number of defects, but once the crystal has been produced the number of defects may change in a way difficult to control, according to the strains or temperatures to which it is submitted -. Thus, the internal defects are considered as internal variables rather than as usual thermodynamic variables. Eq. $(5)_1$ can be simplified, for instance, by assuming for the dislocation flux $\mathscr{V}_{ijk} = -D\frac{\partial a_{ij}}{\partial x_k}$, with D being a diffusion coefficient for dislocations (which could be a fourth-order tensor instead of a simple scalar, but we will not deal with such added complications, because they are not essential to clarify the point we are dealing with in this paper). This is, indeed, the common situation describing diffusion of defects in solids. On the other hand, the production term may be seen as the combination of a dislocation-formation term and a dislocation-destruction term, namely, $A_{ij} = A_{ij}$ (formation) $-A_{ij}$ (destruction).

Then, we consider for the evolution equation for a_{ij} the simple form

$$\frac{da_{ij}}{dt} - D\nabla^2 a_{ij} = A_{ij,eq} + \tilde{\alpha}\tilde{q}_{2i}\tilde{q}_{2j}. \tag{6}$$

Here, $A_{ij,eq}$ is the net formation tensor in the absence of an external energy flux, and we have added to it a tensor depending on the external energy flux $\tilde{\mathbf{q}}_2$ to describe the additional contribution to dislocation formation (for instance, by energetic neutrons).

This form does not pretend to be especially realistic, but only to illustrate that thermal stresses related to $\tilde{q}_{2i}\tilde{q}_{2j}$ could influence the evolution of dislocation lines. More realistic than a simple energy flux, would be to consider, for instance, an energy flux due to the bombardment of the crystal with particles having relatively high energy, which could produce new defects (as point defects, that we will comment in the concluding section, or modify the structure of the dislocation lines). This kind of bombardment is found, as previously said, in anisotropic materials submitted to high radiation fluxes or high fluxes of neutrons in nuclear reactors. Here, in accordance to Restuccia (2016) we will take the linearized expressions

$$\dot{\alpha}_{ij} = \mathscr{V}_{ijk,k} + \beta^1_{ijkl}\varepsilon_{kl} + \beta^2_{ijk}\theta_{neq,k} + \beta^3_{ijkl}\alpha_{kl} + \beta^4_{ijklm}\alpha_{kl,m} + \beta^5_{ijk}q_k + \tilde{A}_{ij}(\tilde{\mathbf{q}}), \tag{7}$$

$$\dot{q}_i = \delta^1_{ijk}\varepsilon_{jk} + \delta^2_{ij}\theta_{neq,j} + \delta^3_{ijk}\alpha_{jk} + \delta^4_{ijkl}\alpha_{jk,l} + \delta^5_{ij}q_j + \tilde{q}_i, \tag{8}$$

where $\beta^i (i = 1,2,...,5)$, $\delta^r (r = 1,2,...,5)$ are assumed constant phenomenological tensors, α_{kl} stands for the non-equilibrium part of the dislocation tensor with respect to an equilibrium reference state a_{kl0},, i. e. $\alpha_{kl} = a_{kl} - a_{kl0}$, and also the other variables stand for deviations referred to an equilibrium state.

We will write (7) and (8) in the simple form

$$\dot{\alpha}_{ij} = D\nabla^2\alpha_{ij} + \beta^1\varepsilon_{ij} - \frac{1}{\tau_1}\alpha_{ij} + \alpha^1\tilde{q}_i\tilde{q}_j, \tag{9}$$

$$\dot{q}_i = -\frac{\lambda}{\tau_2}\theta_{neq,i} + \delta^4\alpha_{kk,i} - \frac{1}{\tau_2}q_i, \tag{10}$$

where τ_1 and τ_2 are the relaxation times. We outline the terms $\alpha^1\tilde{q}_i\tilde{q}_j$ in (9) and $\delta^4\alpha_{kk,i}$ in (10), which present a coupling between the heat flux and the gradient of dislocations. The meaning of the non-equilibrium temperature will be analyzed in the next section. The term in $\delta^4\alpha_{kk,i} (= \delta^4\nabla\rho_D)$ brings a contribution to the flux of dislocations, proportional to $-D\nabla\rho_D$ in its simplest form, to the heat flux. This is intuitive, because if dislocations move they will carry some internal energy. This raises the question of the contribution of the dislocations to the internal energy and to the heat flux, which is related to the temperature of dislocations.

4. Temperature definitions in equilibrium and non-equilibrium thermodynamics

In equilibrium thermodynamics there are several definitions of temperature (Muschik 1989, 1993; Luzzi *et al.* 1997; Casas-Vázquez and Jou 2003): *empirical* (based on the zeroth law), *caloric* (based on the first law), and *entropic* (based on the second law). The caloric one is related to the *energy contents* of the system, whereas the entropic one is related to the capacity of *energy exchange* with other systems. Energy and entropy of interacting dislocations has been worked in detail in Ladd and Hoover (1982), giving concrete expressions which could be useful as explicit illustrations of our work. There are also other definitions based on statistical physics, on fluctuation theory, on fluctuation-dissipation theory, but we will focus our attention on the three mentioned thermodynamic definitions. Temperature in non-equilibrium thermodynamic theories is a relevant challenge when going beyond the local-equilibrium theory (Muschik 1989, 1993; Baranyai 2000; Casas-Vázquez and Jou 2003; Hatano and Jou 2003; Powles *et al.* 2005; Criado-Sancho *et al.* 2006, 2008; Jepps and Rondoni 2010; Jou *et al.* 2010; Jou and Restuccia 2011; Daivis and Jou 2012; Jou and Restuccia 2016). For instance, one may do so on the basis of the internal energy of some degrees of freedom, as the average kinetic energy (kinetic temperature), the average vibrational energy (vibrational temperature), or some averages of the intermolecular potential energy (configurational temperature), or one may start from the Gibbs equation, and relate the temperature to the derivative of the internal energy with respect to the entropy (absolute temperature). One may also explore other definitions, as the relation between entropy flux and heat flux, or the second moments of the fluctuations of the variables, or the Einstein relation between diffusion and particle mobility, and so on.

In equilibrium states, all these definitions lead to the same value for the temperature, but in non-equilibrium steady states they lead to different values. In fact, it may be relatively easier to measure the temperature of a given degree of freedom, by selecting a phenomenon depending on it, than measuring the entropic temperature, which requires a simultaneous control of several degrees of freedom (in principle, of all the variables on which the entropy is assumed to depend). Thus, studying non-equilibrium temperatures, here, we basically aim to identify and define the temperatures of the several degrees of freedom and comment on their difference with respect to the entropic temperature, which is more difficult to measure.

In Criado-Sancho *et al.* (2006) and Criado-Sancho *et al.* (2008) the relation between local-equilibrium temperature, kinetic temperature in the three spatial directions, thermodynamic temperature related to the non-equilibrium entropy, and fluctuation-dissipation temperature has been explicitly obtained in an ideal gas in Couette flow and in mixtures of ideal gases. In Hatano and Jou (2003), it was studied the relation between kinetic temperature and configurational temperature of a forced harmonic oscillator.

4.1. Definitions of temperature. *Empirical definition*:

Empirical (or thermometric) temperature θ_{emp} is defined by the zeroth law, which states the transitive character of thermal equilibrium. In particular, it states that if a state A of a system is in equilibrium with state B of another system, and state B is in equilibrium with state C of a third system, states A and C are in mutual thermal equilibrium.

Entropic definition:

The most fundamental definition of temperature, in equilibrium thermodynamics, is that of absolute temperature, appearing in the Gibbs equation (Jou *et al.* 2004; Jou and Restuccia 2016). Namely

$$\frac{1}{\theta_{eq}} \doteq \left(\frac{\partial S}{\partial U}\right)_{all\ other\ extensive\ variables} . \tag{11}$$

The subscript "all other extensive variables" besides the parenthesis means that the derivative of the total entropy S with respect to the total internal energy U must be carried out keeping constant all the other extensive variables appearing in the entropy, as for instance the volume V, the number of particles N_i of the species i, the total magnetization $\mathbf{M}$, and so on.

Caloric definition:

Another usual definition of temperature T_{eq} - we will call it the caloric definition, because it uses the so-called caloric equation of state relating internal energy and temperature - is obtained from the internal energy U, as for instance

$$U = U(T_{eq}, V, N_i). \tag{12}$$

Since U is defined by the first principle, this definition is related to this principle.

The caloric definition of temperature is used in many situations. These definitions may be generalized to a local version, by considering small volume elements in a given position.

4.2. Non-equilibrium entropic temperature. The entropic definition of non-equilibrium absolute temperature θ_{neq} is related to the Gibbs equation which, for the system we are considering, has the form

$$ds = \theta_{neq}^{-1} du + \theta_{neq}^{-1} \sigma_{ij} d\varepsilon_{ij} - \theta_{neq}^{-1} \pi_{ij} da_{ij} - \theta_{neq}^{-1} \pi_i dq_i, \tag{13}$$

with s the local entropy density per unit mass, π_{ij} the corresponding thermodynamic potential conjugate of the dislocation tensor a_{ij}, π_i the corresponding thermodynamic conjugate of the heat flux q_i, and u is the local total internal energy per unit mass of all the degrees of freedom. In the simplest situations we can assume $u_{dis} = \alpha \rho_D + \beta \rho_D^2$, which in the linear case reduces to $u_{dis} = \alpha \rho_D$, with α the energy per unit length of dislocations.

We suppose that only the internal variable under consideration is modified by the presence of an external energy flow. Of course the classical variables, like u and ε_{ij}, will also be modified by the flux, but here we refer to the modification of temperature for given values of the classical variables, for this reason we will omit these variables in the next expressions.

The definition of equilibrium thermodynamic absolute temperature is given by (11). The same definition is valid out of equilibrium. In steady states θ_{neq}^{-1} can be expanded around its equilibrium counterpart in the following way (neglecting the other first order terms and those of order higher than the first one)

$$\theta_{neq}^{-1} = \theta_{eq}^{-1} - \theta_{eq}^{-2} \frac{\partial \theta_{eq}}{\partial a_{ij}} \Delta a_{ij}, \tag{14}$$

where in steady states

$$\Delta a_{ij} = a_{ij}(\tilde{\mathbf{q}} \neq 0) - a_{ij}(\tilde{\mathbf{q}} = 0). \tag{15}$$

More realistically, we consider, for instance, an energy flux due to the bombardment of the crystal with particles having relatively high energy such to modify the structure of the dislocation lines or to produce new dislocations but not to influence the physical fields described by the other variables, and such that the new thermodynamic state rests around its equilibrium counterpart.

Then, in the first approximation, the non-equilibrium temperature θ_{neq} will be related to the equilibrium temperature corresponding to a_{ij} $(\tilde{\mathbf{q}} = 0)$ as

$$\theta_{neq} = \frac{\theta_{eq}}{1 - \theta_{eq}^{-1} \frac{\partial \theta_{eq}}{\partial a_{ij}} \Delta a_{ij}} \approx T_{eq} \left(1 + T_{eq}^{-1} \left(\frac{\partial T_{eq}}{\partial a_{ij}} \right) \Delta a_{ij} \right) =$$

$$T_{eq} + \left(\frac{\partial T_{eq}}{\partial a_{ij}} \right) \Delta a_{ij}, \tag{16}$$

where we have taken into account that in equilibrium (or local-equilibrium) all the definitions of temperature coincide, therefore $\theta_{eq} = T_{eq}$, and we have used the approximation

$$(1-x)^{-1} \approx 1 + x,$$

for $x \ll 1$.

4.3. Non-equilibrium caloric temperature. To define the caloric definition of non-equilibrium temperature related to the dislocation field first we consider the caloric equation of state at the equilibrium of the system for given values of ε_{kl} and the other fields, and for vanishing values of the external neutron flux $\tilde{\mathbf{q}}$ and the heat flux $\mathbf{q}$:

$$u_{dis} = U \left(a_{ij}(T_{eq}, \varepsilon_{kl}), T_{eq}, \varepsilon_{kl} \right), \tag{17}$$

where we have called u_{dis} the internal energy corresponding to dislocations and we have taken in consideration that at equilibrium the internal variable depends on temperature and the stress tensor. Then, we define the caloric non-equilibrium temperature field T_{neq} related to a_{ij} in a steady state in the following way

$$u_{dis} \left(a_{ij}(T_{neq}, \varepsilon_{kl}, \tilde{\mathbf{q}} = 0), T_{neq}, \varepsilon_{kl} \right) \doteq u_{dis} \left(a_{ij} \left(T_{eq}, \varepsilon_{kl}, \tilde{\mathbf{q}} \right), T_{eq}, \varepsilon_{kl} \right). \tag{18}$$

Then, to define the caloric non-equilibrium temperature assume that the formal expression of the relation between the internal energy U_{dis} and temperature keeps, out of equilibrium, the same form as in equilibrium (see (16)), where $\tilde{\mathbf{q}} = 0$, and we equate it to the value of the internal energy u_{dis} in non-equilibrium, where $\tilde{\mathbf{q}} \neq 0$. Thus, we define the temperature in non-equilibrium state as that temperature which, introduced in the caloric state equation would give for the internal energy u_{dis} the actual value corresponding to the non-equilibrium state. Namely, we will have, in the same approximation as in subsection 3.1,

$$T_{neq} = T_{eq} + \left(\frac{\partial T_{eq}}{\partial u_{dis}} \right) \Delta u_{dis} = T_{eq} + \left(\frac{1}{c_{dis}} \right) \Delta u_{dis}, \tag{19}$$

where $\left(\frac{\partial T}{\partial U_{dis}} \right) \Delta u_{dis}$ is the non-equilibrium contribution due to the presence of $\tilde{\mathbf{q}} \neq 0$, and c_{dis} is the specific heat associated to the changes of the internal energy of dislocation lines, per unit volume, namely $c_{vdis} = \frac{\partial u_{dis}}{\partial T_{eq}}$. The specific heat plays thus an important role in the caloric definition of temperature.

Now, we will see that in this order of approximation both definitions (16) and (19) coincide. In fact, expression (16) may also be written, using (18), as

$$\theta_{neq} = T_{eq} + \left(\frac{\partial T_{eq}}{\partial u_{dis}} \right) \left(\frac{\partial u_{dis}}{\partial a_{ij}} \right) \Delta a_{ij} = T_{eq} + \left(\frac{\partial T_{eq}}{\partial u_{dis}} \right) \Delta u_{dis}, \tag{20}$$

with Δu_{dis} being $\Delta u_{dis} = \left(\frac{\partial u_{dis}}{\partial a_{ij}}\right)\Delta a_{ij}$. Thus, both definitions of non-equilibrium temperature are equal.

5. Entropic flux in the definition of non-equilibrium temperature

It is logical to expect that the entropy flux $\mathbf{J}^S$ will depend not only on heat flux, but also on the dislocation flux. Indeed, in Restuccia (2019) it was seen that in the case of a crystal with dislocations, the entropy flux has the form

$$J_k^S = \theta_{neq}^{-1} q_k - \pi_{ij}\theta_{neq}^{-1}\mathcal{V}_{ijk}. \tag{21}$$

Here, the variable π_{ij} is the conjugate to a_{ij} as introduced in (13). Eq. (21) is a natural generalization of the expression for the heat flux in multicomponent systems, which is

$$J_k^S = \theta^{-1} q_k - \sum_{\alpha=1}^{n} \theta^{-1}\mu_\alpha J_k^\alpha, \tag{22}$$

with μ_α being the chemical potential of the chemical species $(\alpha = 1, 2, ..., n)$ and $\mathbf{J}^\alpha$ the flux of species α. Dislocations may be interpreted in this setting as a “tensorial ” chemical component.

It has been proposed that a convenient definition of a non-equilibrium contribution could be based on expression (21), taking as the reciprocal of thermodynamic temperature the coefficient linking the heat flux $\mathbf{q}$ with the entropy flux $\mathbf{J}^S$ (Müller 1971; Jou *et al.* 2004). Based on the assumption of perfect interfaces between systems, in which both the heat flux and the entropy flux would be continuous, M*ü*ller based on this idea the definition of the so-called "“coldness” namely, of the reciprocal of absolute temperature (Müller 1971).

Considering the entropy flux and the heat flux through an interface between two systems (let us say, a thermometer and a system) is convenient, because this reminds us the importance of the contact between the system and the thermometer in measuring temperature.

In this aspect, problematic questions arise. In first place, the existence of ideal interfaces is a nice theoretical concept, but in general the interfaces between different materials are not ideal, but exhibit the so-called “thermal boundary resistance”, which implies a discontinuity of temperature trough the surface, and a corresponding discontinuity of the entropy flux, due to entropy production across the wall, due to the fact that heat is flowing between two different temperatures. Finally, a last precaution in considering the relation between heat flux and entropy flux as a way to define temperature, is that one must be sure that only heat flux is exchanged between the two systems separated by the interface, but not other quantities - nor matter, nor dislocations, for instance. Otherwise, if there is a dislocation flux between the systems, the observed entropy flow will be related to the heat flux in a way different than when heat flux is the only exchange, as studied in Restuccia (2019), in the framework of the extended irreversible thermodynamics, where the heat and dislocation fluxes are introduced in the state space as independent variables besides the local temperature θ_{neq}, the local strain tensor ε_{ij} and the dislocation tensor a_{ij}. To simplify the presentation, we may assume that we have a vectorial dislocation flux $\mathbf{J}_{dis}$, related to the tensorial flux V_{ijk} mentioned in Section 3 as $V_{ijk} = J_i\delta_{jk} + J_k\delta_{ij} + J_j\delta_{ik}$, δ_{ij} being Kronecker’s delta. Also, in some occasions, one has that $\mathbf{J}_{dis} = -\lambda_v\mathbf{q}$, and the relation (21) becomes

$$J_i^S = \theta^{-1} q_i - \theta^{-1}\pi_{ij}J_{dis\,j} = \theta^{-1}(1 + \pi\lambda_v)q_i, \tag{23}$$

where we have assumed that the tensor π_{ij} reduces to $\pi\delta_{ij}$, for the sake of simplicity. Relation (23) would lead to a different relation between entropy flux and heat flux. Thus, it is clear that considering the entropy flux is useful, at least, to have a better understanding on the relevance of exchanging only heat flow in order to have a good evaluation of the temperature.

6. Final comments and conclusions

In this paper we have emphasized three relevant aspects of dislocation non-equilibrium thermodynamics: the influence of dislocations on thermal conductivity, which is a topic of much direct practical interest, which may be mathematically stated as

$$\mathbf{q}_{ss} = -\lambda(\alpha_{ij})\nabla T, \tag{24}$$

and two topics of more fundamental character: the contribution of dislocation flux to the heat flux, and the caloric and entropic temperatures of dislocations. The caloric temperature is related to the energy stored in dislocation lines, which may be a considerable amount of energy, thus leading to caloric temperature much higher than kinetic and potential temperatures of the lattice. However, this energy will be exchanged very slowly with the lattice, because of a very small energy transfer coefficient. If the variable α_{ij} depends, according to (6), on the heat flux, Eq. (24) may become a highly non-linear equation. Therefore, even in the case in which the internal variables did not partecipate directly in the heat flow, they could have a strong influence on it through their influence on the thermal conductivity. For instance, a heat flux, which is associated to temperature gradient, could produce a differential stress on the dislocations as a consequence of a differential of thermal expansion in hotter and colder regions. This could induce a drift motion of dislocations from one region to the other, thus provoking modifications in the thermal conductivity. This could be also produced, of course, by a differential stress of mechanical origin.

Appendix: A dislocation core tensor model

The dislocation lines disturb the periodicity of the lattice of the crystal and their structure resembles a network of infinitesimally thin channels. These defects can self propagate, because of changed and favorable surrounding conditions. They have their intrinsic orientation, which means, among others, that two dislocations of opposite signs annihilate when lines close to each other. Here, we introduce a dislocation core à la Maruszewski (Kubik 1986; Maruszewski 1991) and its gradient in the thermodynamical state space of independent variables for describing these defects.

A representative elementary sphere volume Ω is considered of a structure with dislocations (see Fig.2), large enough to provide a representation of all the statistical properties of the channel space Ω^{ch}. Then, we have: $\Omega = \Omega^{s} + \Omega^{ch}$, where Ω^{s} is the solid space. We assume that the coefficient $f_v = \frac{\Omega^{ch}}{\Omega}$ remains constant inside the medium. All the microscopic quantities are described with respect to the ξ_i coordinate system $(i = 1,2,3)$, while macroscopic quantities are described with respect to the x_i axes $(i = 1,2,3)$. Let $\alpha(\xi)$ be any scalar, vector or second order tensor which represents some microscopic property of the flux of some physical field flowing through the channel space Ω^{ch} and related to a coordinate system ξ_i. We assume that such quantity is zero in the solid space Ω^{s}.

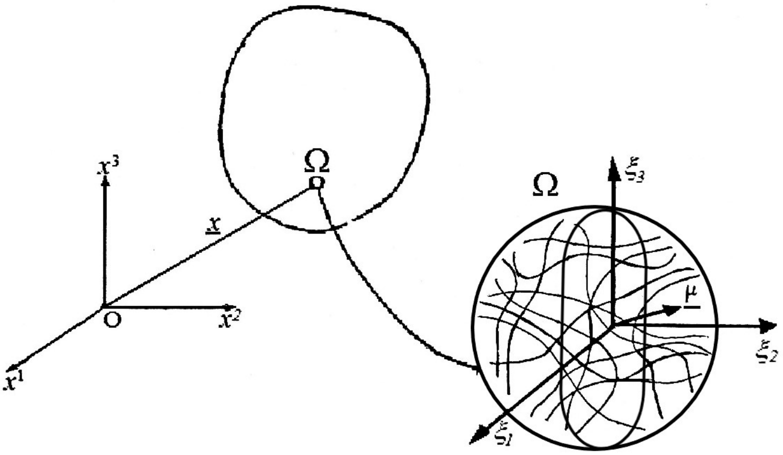

FIGURE 2. Characteristics of a structure with dislocations.

The volume averaging procedures give (Kubik 1986; Maruszewski 1991)

$$\hat{\alpha}(\mathbf{x})=\frac{1}{\Omega^{ch}}\int_{\Omega^{ch}}\alpha(\xi)d\Omega, \qquad \bar{\alpha}(\mathbf{x})=\frac{1}{\Omega}\int_{\Omega^{ch}}\alpha(\xi)d\Omega, \tag{25}$$

where the quantities $\hat{\alpha}(\mathbf{x})$, $\bar{\alpha}(\mathbf{x})$ (related to the coordinated system x_i) describe the property of the flux of the physical field under consideration at macroscopic level. They are averaged quantities on the channel-volume and on the bulk-volume, respectively. Similarly, we define the averaged quantity $\overset{*}{\alpha}(\mathbf{x})$ on the channel-area as follows

$$\overset{*}{\alpha}(\mathbf{x};\mu)=\frac{1}{\Gamma^{ch}}\int_{\Gamma^{ch}}\alpha(\xi)d\Gamma, \tag{26}$$

where Γ is the central sphere section and Γ^{ch} represents the channel-area of Γ. The orientation of Γ in Ω is given by the normal vector μ. Thus, $\Gamma=\Gamma^s+\Gamma^{ch}$, where Γ^s is the solid area. By definition the quantity $\alpha(\xi)$ is zero on the solid-surface Γ^s. In such a medium Maruszewski defines the so called dislocation tensor, as follows

$$\bar{\alpha}(\mathbf{x})_i=r_{ij}(\mathbf{x},\mu)\,\overset{*}{\alpha}_j(\mathbf{x},\mu). \tag{27}$$

Eq. (27) gives a linear mapping between an averaged quantity on the bulk volume and the average of the same quantity on the channel area. Furthermore, Maruszewski introduces a new tensor a_{ij}, that refers r_{ij} to the central sphere section Γ and is defined in the following way

$$a_{ij}(\mathbf{x},\mu)=\Gamma^{-1}r_{ij}(\mathbf{x},\mu). \tag{28}$$

a_{ij} is called *dislocation core tensor* and has unit m^{-2} (Maruszewski 1991).

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