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Thermodynamics of extrinsic semiconductors with dislocations

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In this paper we construct a geometric model for the thermodynamics of deformable semiconductors with impurities defective by dislocations, using a nonconventional model based on the extended irreversible thermodynamics with internal variables developed in [1], in which a dislocation density tensor *à* la Maruszewski (see Fig.1, 2 and 3) and its flux are introduced as internal variables. The dislocation lines disturb the periodicity of the lattice of the crystal and their structure resembles a network of infinitesimally thin pores or capillary tubes . Following [2], we introduce the concepts of *processes* and *transformations* and we derive the entropy function. The models for semiconductors defective by dislocations may have relevance in in many fundamentals technological sectors: in applied computer science, in the technology for integrated circuits VLSI (Very Large Scale Integration), in the field of electronic microscopy, in the nanotechnology. The defects acquired during the process of fabrication can provoke a premature fracture because they can self propagate because of changed conditions and surrounding conditions that are favorable. Now, we recall the model developed in [1], where it was assumed that in anelastic and defective semiconductor the following fields interact with each other: *the elastic field* described by the stress tensor T_{ij} and the small-strain tensor ε_{ij}; *the thermal field* described by the temperature θ and the heat flux q_i; *the electromagnetic field* described by the electromotive intensity $\mathcal{E}_i$ and the magnetic induction B_i; *the charge carrier fields* described by the densities of electrons n and holes p and their fluxes j_i^n and j_i^p, respectively; *the dislocation field* described by the dislocation density tensor a_{ij} and the dislocation flux $\mathcal{V}_{ijk}$. The independent constitutive variables are represented by the set

$$C = \{\varepsilon_{ij}, \mathcal{E}_i, B_i, n, p, \theta, a_{ij}, \mathcal{V}_{ijk}, j_i^n, j_i^p, q_i, n_{,i}, p_{,i}, \theta_{,i}, a_{ij,k}\}\,. \tag{1}$$

All the processes occurring in the body considered are governed by the following laws:
the continuity equation: $\dot{\rho} + \rho v_{i,i} = 0$,
where ρ denotes the mass density, the superimposed dot denotes the material derivative and the mass charge carriers have been neglected compared to ρ;
the momentum balance: $\rho \dot{v}_i - T_{ji,j} - \rho Z \mathcal{E}_i - \varepsilon_{ijk}\left(j_j^n + j_j^p + \overset{\triangle}{P}_j\right) B_k - P_j \mathcal{E}_{i,j} - f_i = 0$,

where $\overset{\triangle}{P}_i = \dot{P}_i + P_i v_{k,k} - P_k v_{i,k}$, $\mathcal{E}_i = E_i + \varepsilon_{ijk} v_j B_k$, the total charge and current are as follows: $Z = n + \bar{n} - n_0 + p + \bar{p} - p_0$, $j_i = j_i^n + j_i^p$, T_{ij} denotes the total stress tensor, P_i is the polarization vector, f_i is the body force (neglected in the following), $n < 0$, $n_0 < 0$, $p > 0$, $p_0 > 0$ denote mass densities of nonequilibrium and equilibrium electrons and holes, respectively, $\bar{n} < 0$ and $\bar{p} > 0$ denote fixed charges of ionized impurities; *the momentum of momentum balance*: $\varepsilon_{ijk} T_{jk} + c_i = 0$.
In [1] it was demonstrated that the coupled c_i for unit volume is vanishing;
the internal energy balance

$$\rho \dot{e} - T_{ji} v_{i,j} - \left(j_j^n + j_j^p \right) \mathcal{E}_j - \rho \mathcal{E}_i \dot{\mathcal{P}}_i + q_{i,i} - \rho r = 0 \tag{2}$$

Here e is the internal energy density, r is the heat source distribution neglected in the follows, $P_i = \rho \mathcal{P}_i$, $v_{i,j} = L_{ij} = L_{(ij)} + L_{[ij]}$ (where $L_{(ij)}$ and $L_{[ij]}$ are respectively the symmetric and antisymmetric part of the velocity gradient and $L_{[ij]} = \Omega_{ij} = \frac{1}{2}(v_{i,j} - v_{j,i})$). Introducing the deformation gradient $\mathbf{F}$, also we have $\mathbf{L} = \nabla \mathbf{v} = \dot{\mathbf{F}} \mathbf{F}^{-1}$.
The electromagnetic field is governed by the following *Maxwell's equations* :

$$\varepsilon_{ijk} E_{k,j} + \frac{\partial B_i}{\partial t} = 0, \quad D_{i,i} - \rho Z = 0, \quad \varepsilon_{ijk} H_{k,j} - j_i - \rho Z v_i - \frac{\partial D_i}{\partial t} = 0, \quad + B_{i,i} = 0,$$

where $H_i = \frac{1}{\mu_0} B_i$, $E_i = \frac{1}{\varepsilon_0} \left(D_i - P_i \right)$, and ε_0, μ_0 denote the permittivity and permeability of vacuum. $\mathbf{H}$ and $\mathbf{D}$ are respectively the magnetic field and the electric displacement field.
The *evolution equations of charge carriers* read: $\rho \dot{n} + j_{i,i}^n - g^n = 0$, $\rho \dot{p} + j_{i,i}^p - g^p = 0$, then *the equations for the ionized impurities* are as follows: $\rho \dot{\bar{n}} = \bar{g}^n$, $\rho \dot{\bar{p}} = \bar{g}^p$, g^n and g^p describe the recombination of electrons and holes and together with the ionization of impurities $\bar{g}^n$ and $\bar{g}^p$ satisfy the equation $g^n + g^p + \bar{g}^n + \bar{g}^p = 0$. Following [1], we take that $\dot{\bar{n}} = \dot{\bar{p}} = 0$ and $\bar{g}^n = \bar{g}^p = 0$.
Further, we have the *evolution equation for the dislocation density*:

$$\overset{*}{a}_{ij} + \mathcal{V}_{ijk,k} - A_{ij}(C) = 0, \quad \text{where} \quad \overset{*}{a}_{ij} = \dot{a}_{ij} - \Omega_{ik} a_{kj} - \Omega_{jk} a_{ik};$$

the *evolution equation for the dislocation flux*:

$$\overset{*}{\mathcal{V}}_{ijk} - \mathcal{V}_{ijk}(C) = 0, \quad \text{where} \quad \overset{*}{\mathcal{V}}_{ijk} = \dot{\mathcal{V}}_{ijk} - \Omega_{il} \mathcal{V}_{ljk} - \Omega_{jl} \mathcal{V}_{ilk} - \Omega_{kl} \mathcal{V}_{ijl}$$

and the *evolution equations* concerning *heat, electron* and *hole fluxes*:

$$\overset{*n}{j}_i - J_i^n(C) = 0, \qquad \overset{*p}{j}_i - J_i^p(C) = 0, \qquad \overset{*}{q}_i = Q_i(C),$$

where $\overset{*n}{j}_i = \dot{j}_i^n - \Omega_{ik} j_k^n$, $\overset{*p}{j}_i = \dot{j}_i^p - \Omega_{ik} j_k^p$, $\overset{*}{q}_i = \dot{q}_i - \Omega_{ij} q_j$.
In the above equations a superimposed asterisk indicates the Zaremba-Jaumann time derivative. All the admissible solutions of the proposed evolution equations should be restricted by the following *entropy inequality*: $\rho \dot{S} + J_{S_{k,k}} - \frac{\rho r}{T} \geq 0$,
where S denotes the entropy per unit mass and $\mathbf{J}_S$ is the entropy flux associated with the fields of the set C given by

$$\mathbf{J}_S = \frac{1}{\theta} \mathbf{q} + \mathbf{k}, \tag{3}$$

with $\mathbf{k}$ an additional term called *extra entropy flux density.*
In [1] all the following constitutive functions $\mathbf{Z} = \tilde{\mathbf{Z}}(C)$ with

$$Z = \{T_{ij}, P_i, c_i, e, g^n, g^p, A_{ij}, V_{ijk}, J_i^n, J_i^p, Q_i, S, \Phi_i, \mu^n, \mu^p, \pi_{ij}\} \tag{4}$$

were obtained by analyzing the entropy inequality by Liu's theorem and (using Smith theorem) with the help of the isotropic polynomial representations of the proper constitutive functions, satisfying the objectivity principle. Now, we construct a geometric model for the thermodynamics of extrinsic defective semiconductors (following [2]) and we derive the expressions for the existence of an entropy function. We assume that the body $\mathcal{B}$ having a regular boundary $\delta\mathcal{B}$, is regularly embedded into Euclidean space $\mathbb{R}^3$ by a regular family of instantaneous time-dependent configurations $\mathcal{B}_t$. We treat the time on equal footing as the other state variables entering explicitly the state functions. Then, we consider a material element and we define the state space at time t as the set B_t of all state variables which "fit" the configuration of the element at time t. B_t is assumed to have the structure of a finite dimensional manifold. The "total state space" is the disjoint union $\tilde{\mathcal{B}} = \bigcup_t \{t\} \times B_t$ with a given natural structure of fibre bundle over $\mathbb{R}$ where time flows [2]; if the instantaneous state space B_t does not vary in time the state space $\tilde{\mathcal{B}}$ reduces to a Cartesian product $\mathbb{R} \times B$. Moreover we consider an abstract space of *processes* [2], i.e. a set Π of functions $P_t^i : [0,t] \to \mathcal{G}$, where $[0,t]$ is any time interval, the space $\mathcal{G}$ being a suitable target space defined by the problem under consideration, i a label ranging in an unspecified index set for all allowed processes and $t \in \mathbb{R}$ the so called *duration* of the process. A continuous function then is defined $\rho : \mathbb{R} \times \Pi \to C^0(B_0, B_t)$ so that for any instant of time t and for any process $P_t^i \in \Pi$ a continuous mapping called *transformation* (induced by the process) is generated. Now, we assume that the behavior of defective thermoelastic semiconductors is described by the following state variables $\mathbf{C} = \{F_{ij}, D_i, B_i, n, p, e, a_{ij}, \mathcal{V}_{ijk}, j_i^n, j_i^p, q_i, n_{,i}, p_{,i}, \theta_{,i}, a_{ij,k}\}$. The full state space is then $\Sigma = Lin(\mathcal{V}) \oplus \mathcal{V} \oplus \mathcal{V} \oplus \mathbb{R} \oplus \mathbb{R} \oplus \mathbb{R} \oplus \mathcal{W}_1 \oplus \mathcal{W}_2 \oplus \mathcal{V} \oplus \mathcal{V} \oplus \mathcal{V} \oplus \mathcal{V} \oplus \mathcal{V} \oplus \mathcal{V} \oplus Lin(\mathcal{W}_1)$, where $\mathcal{V} \simeq \mathbb{R}^3$, W_1 and W_2 are vector spaces accounting for the internal variables $\mathbf{a}$ and $\mathcal{V}$ respectively. The process P_t^i is described by the following functions

$$P_t^i = [\mathbf{L}, \boldsymbol{\mathcal{H}}, \boldsymbol{\Xi}, G^n, G^p, h, \boldsymbol{\gamma}, \boldsymbol{\Lambda}, \boldsymbol{\mathcal{J}}^n, \boldsymbol{\mathcal{J}}^p, \boldsymbol{\mathcal{Q}}, \boldsymbol{\mathcal{N}}, \boldsymbol{\mathcal{P}}, \boldsymbol{\Theta}, \boldsymbol{\Gamma},], \tag{5}$$

where $\mathcal{H}_i = \epsilon_{ijk} H_{k,j} - (j_i^n + j_i^p) - \rho \mathcal{Z} v_i$; $\quad \Xi_i = -\epsilon_{ijk} E_{k,j}$; $\quad G^n = g^n - j_{i,i}^n$;
$G^p = g^p - j_{i,i}^p$; $\quad h = (j_i^n + j_i^p)\mathcal{E}_i - \frac{\dot{\rho}}{\rho}\mathcal{E}_i P_i + \mathcal{E}_i \dot{P}_i - q_{i,i} + \rho r$; $\quad \gamma_{ij} = \Omega_{ik} a_{kj} - a_{ik}\Omega_{kj} - \mathcal{V}_{ijk,k} + A_{ijk}$; $\quad \Lambda_{ijk} = \Omega_{il}\mathcal{V}_{ljk} + \Omega_{jl}\mathcal{V}_{ilk} + \Omega_{kl}\mathcal{V}_{ijl} + V_{ijk}$; $\quad \mathcal{J}_i^n = J_i^n + \Omega_{ik} j_k^n$; $\quad \mathcal{J}_i^p = J_i^p + \Omega_{ik} j_k^p$;
$\mathcal{Q}_i = Q_i + \Omega_{ik} q_k$.
Following standard procedures in this geometrical structure we are able to introduce an "entropy function", which is related to a transformation between the initial and the actual states σ_0 and σ_t, by setting [2]:

$$s(t) = -\int_0^t \frac{1}{\rho} \nabla \cdot \mathbf{J}_S d\tau, \tag{6}$$

where $\mathbf{J}_S$ is defined according to equation (3). We assume that the transformations

induced by the process are governed by the following dynamical system

$$\begin{cases} \dot{\mathbf{F}} &= \mathbf{L}(\tau)\mathbf{F}(\tau) \\ \dot{\mathbf{D}} &= \boldsymbol{\mathcal{H}}(\tau) \\ \dot{\mathbf{B}} &= \boldsymbol{\Xi}(\tau) \\ \rho\dot{n} &= G^n(\tau) \\ \rho\dot{p} &= G^p(\tau) \\ \rho\dot{e} &= \mathbf{T}(\sigma)\cdot\mathbf{L}(\tau) + h(\tau) \\ \dot{\mathbf{a}} &= \boldsymbol{\gamma}(\tau) \\ \dot{\mathcal{V}} &= \boldsymbol{\Lambda}(\tau) \\ \dot{\mathbf{j}}^n &= \boldsymbol{\mathcal{J}}^n(\tau) \\ \dot{\mathbf{j}}^p &= \boldsymbol{\mathcal{J}}^p(\tau) \\ \dot{\mathbf{q}} &= \boldsymbol{\mathcal{Q}}(\tau) \\ \dot{\nabla n} &= \boldsymbol{\mathcal{N}}(\tau) \\ \dot{\nabla p} &= \boldsymbol{\mathcal{P}}(\tau) \\ \dot{\nabla\theta} &= \boldsymbol{\Theta}(\tau) \\ \dot{\nabla\mathbf{a}} &= \boldsymbol{\Gamma}(\tau). \end{cases} \tag{7}$$

Then we get an expression for s(t) which in turn defines a 1-form Ω in $\mathbb{R}\times B$ called the *entropy 1-form* in the following way: $s=\int_\sigma \Omega$. Using Eqs. $(7)_6$, (3) we obtain

$$\begin{aligned} \Omega = &-\tfrac{1}{\rho\theta}\mathbf{T}\mathbf{F}^{-T}d\mathbf{F} - \tfrac{1}{\rho\theta}(\mathbf{E}+\mathbf{v}\wedge\mathbf{B})\cdot d\mathbf{D} + \tfrac{1}{\theta}de + \\ &\Big[\tfrac{1}{\rho\theta^2}\mathbf{q}\cdot\nabla\theta - \tfrac{1}{\rho\theta}(\mathbf{j}^n+\mathbf{j}^p)\cdot(\mathbf{E}+\mathbf{v}\wedge\mathbf{B}) + \tfrac{1}{\rho\theta^2}\dot{\rho}(\mathbf{E}+\mathbf{v}\wedge\mathbf{B})\cdot\mathbf{P} + \\ &\tfrac{\varepsilon_0}{\rho\theta}(\mathbf{E}+\mathbf{v}\wedge\mathbf{B})\cdot\dot{\mathbf{E}} - \tfrac{1}{\rho}\nabla\cdot\mathbf{k}\Big]\, d\tau, \end{aligned} \tag{8}$$

where the expressions for $\mathbf{T}$, $\mathbf{P}$, $\mathbf{k}$, $\mathbf{j}^n$, $\mathbf{j}^p$ and $\mathbf{q}$ have been calculated in [1] in a suitable form, Thus the entropy function is now calculated as an integral along a path into the space $\mathbb{R}\times B$ of all thermodynamic variables together with the independent time variable. Finally, by applying the closure conditions for the 1-form we give the necessary conditions for the existence of the entropy function during analyzed processes.

References

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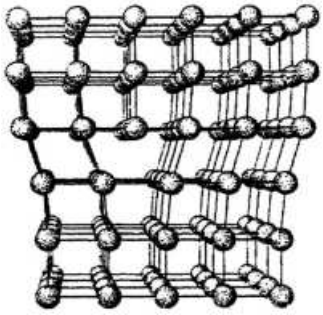

Fig.1 An edge dislocation structure (see [1]).

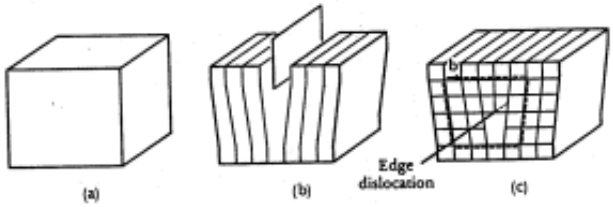

Fig.2 The perfect crystal in (a) is cut and an extra plane of atoms is inserted; in (b) the bottom edge of the extra plane is an edge dislocation ; in (c) a *Burgers vector* is required to close a loop of equal atom spacings around the edge dislocation (see [1]).

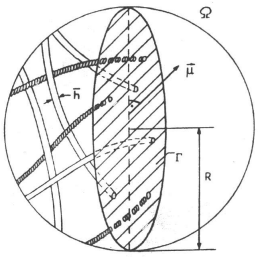

Fig.3 Characteristics of the pore-core structure ($\bar{h} \ll R$) (see [1]).