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Strain Effects in Semiconductors

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Résumé — While it has been known, for long, that mechanical strains affect the electronic behavior of semiconductors, both the theoretical aspects of the coupling between mechanics and electronics and their practical consequences on the response of semiconductor devices remain to be investigated. In this work, we first develop a general fully-coupled mechanical, electrical and electronic continuum model of the finitely deformable semiconductor and subsequently use it to compute the strain-induced changes in the current-voltage characteristic of a *p-n* junction subjected to bending.

Mots clés — semiconductors, chemical potential, electromechanical process.

1 Introduction

Mechanical effects play an important role in semiconductor physics, as first discovered by Bardeen and Shockely [1] and subsequently utilized in several applications (e.g. piezoresistors [2], strained MOS-FET [4]). Different aspects of the coupling between the mechanical and electronic responses of semiconductors have been investigated by the solid-state physics and mechanics communities. The first community is essentially interested in scale bridging, i.e. predicting influence of strain on macroscopic properties based on the electronic band structure. The second group, using ideas of continuum mechanics and thermodynamics, has developed theoretical models of the coupled electro-mechanical problem. The goal of the present work is to derive, using ideas from solid-state physics, a consistent fully-coupled continuum model of the finitely deformable semiconductor. Subsequently and motivated by photovoltaics application we use this model to solve the *p-n* junction under strain gradient.

In the solid-state physics community, starting with the work of Bardeen and Shockley [1], theoretical studies addressed the effect of strain on the band structure of a semiconductor. The modifications of the electronic band structure due to mechanical strains induces changes in the electronic properties of semiconductors (band edge energy level, densities of states, mobilities ; see e.g. [10, 3, 8]).

By contrast, in the mechanics community, the approach consists in modeling semiconductors as a continuum, by writing a boundary value problem that involves the mechanical, electrostatic and electronic fields *which mutually interact*. This is what has been done by de Lorenzi and Tiersten [7], who developed a theory of the fully coupled problem where the unknown fields consist of the strain field for the mechanics, the electromagnetic field, and the free carriers distributions for the electronics. However, in this work, no explicit form is given for the constitutive relations, which make it difficult to establish a connection with the governing equations used in semiconductor physics.

In the present work, we derive, in Sec. 2, a fully-coupled electrostatic-electronic-mechanical theory of deformable semiconductors. We use a consistent treatment of the interaction of the electric field with polarizable matter [11] and of the thermodynamic modeling of charge carriers transports [9]. Specializing to crystalline semiconductors and using results of mechanics, electromagnetism and statistical physics, a functional form of the free energy — from which the constitutive laws derive — is proposed.

Following the development of the general theory, we give, in Sec. 3, an application were strain nonuniformity plays an essential role. Motivated by the strain effects on the performances of a photovoltaic cells, we compute, using asymptotic methods, the current-voltage response of a *p-n* junction subjected to nonuniform strains which result from bending.

2 Continuum formulation for deformable semiconductors

In this section, we derive the field governing equations that describe the mechanical, electromagnetic and electronic states of a finitely deformable semiconductor.

2.1 Description of the semiconductor

The semiconductor consists of a continuum with electrons donors and electrons acceptors impurities rigidly bound to the continuum with concentrations $N_d(\mathbf{x},t)$ and $N_a(\mathbf{x},t)$ respectively. This induces a volume charge density $q\rho C$ where q is the elementary charge, ρ the mass density and $C(\mathbf{x},t)$ is defined by

$$C := N_d - N_a.$$

Charge transport in the semiconductor occurs through free carriers, which consist of two entities : electrons (of charge $-q$) and holes (of charge q), with concentrations $n(\mathbf{x},t)$ and $p(\mathbf{x},t)$. Electrons and holes are freely moving in the conduction and valence bands respectively. The resulting charge density reads

$$q\rho(C + p - n).$$

In addition to the spatial motion of electrons and holes within their bands, there is possibility for an electron to locally jump between the valence and conduction bands, which is represented by a recombination-generation rate $R(\mathbf{x},t)$ of the electron-hole pairs. The electric displacement $\mathbf{d}(\mathbf{x},t)$, electric field $\mathbf{e}(\mathbf{x},t)$ and polarization $\mathbf{P}(\mathbf{x},t)$ are related by

$$\mathbf{d} = \varepsilon_0 \mathbf{e} + \rho \mathbf{P},$$

where ε_0 is the vacuum permittivity. We ignore all the magnetic fields (magnetic field, magnetic induction, magnetization).

The kinematic description of the deformable medium follows standard mechanics notation : A material point at position $\mathbf{X}$ in the reference configuration is mapped at time t to the spatial point $\mathbf{x} = \chi(\mathbf{X},t)$.

2.2 General principles

The system evolution follows the general principles of the different physics involved. We write the local form of these laws that can be derived from balances on control volumes.

For the electrostatic, we write the Gauss's law

$$\nabla \cdot \mathbf{d} = q\rho(C + p - n),$$

and make use of the Maxwell Faraday's law to write the electric field as the gradient of the electric potential $\phi(\mathbf{x},t)$

$$\mathbf{e} = -\nabla\varphi.$$

Denoting by $\mathbf{j}_n(\mathbf{x},t)$ and $\mathbf{j}_p(\mathbf{x},t)$ the electrons and holes current densities, the balance of free carriers reads

$$\rho\dot{n} = -R - \nabla \cdot \mathbf{j}_n,$$
$$\rho\dot{p} = -R - \nabla \cdot \mathbf{j}_p.$$

For the mechanical description, following the approach of Kovetz [11], we introduce the total Cauchy stress tensor $\boldsymbol{\sigma}(\mathbf{x},t)$ whose associated traction $\mathbf{t} = \mathbf{n} \cdot \boldsymbol{\sigma}$ accounts for the mechanical and electrostatic force density. The balance of mass, balance of linear momentum and balance of angular momentum yield

$$\dot{\rho} + \rho(\nabla \cdot \dot{\mathbf{x}}) = 0,$$
$$\rho\ddot{\mathbf{x}} = \nabla \cdot \boldsymbol{\sigma} + \rho\mathbf{f},$$
$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T.$$

where $\mathbf{f}(\mathbf{x},t)$ is the purely mechanical specific body force.

The coupling of the different phenomena appears in the thermodynamics principles : energy balance and entropy imbalance which combine to a free-energy imbalance. By introducing the free-energy density

$$\psi := u - \theta\eta - \frac{\varepsilon_0}{2\rho}\mathbf{e} \cdot \mathbf{e},$$

where θ is the temperature; u and η are the specific internal energy and entropy respectively, the free-energy imbalance reads

$$\rho(\dot{\psi} + \eta\dot{\theta}) + \left[-\boldsymbol{\sigma} + \mathbf{de} - \frac{\varepsilon_0}{2}(\mathbf{e} \cdot \mathbf{e})\mathbf{I} \right] \cdot\cdot(\dot{\mathbf{x}}\nabla) - \rho\mathbf{e} \cdot \dot{\mathbf{P}} - \rho(\mu_n\dot{n} + \mu_p\dot{p})$$
$$+ \nabla(\mu_n - q\varphi) \cdot \mathbf{j}_n + \nabla(\mu_p + q\varphi) \cdot \mathbf{j}_p - (\mu_n + \mu_p)R + \frac{1}{\theta}\mathbf{q} \cdot (\nabla\theta) \leq 0. \quad (1)$$

where μ_n and μ_p are the chemical potentials associated to electrons and holes respectively.

2.3 Constitutive relations

Following the Coleman-Noll procedure [5], extended by Kovetz [11] and Gurtin [9] for including electromagnetism and species transport respectively, we place restrictions on the constitutive relations. Assuming a dependence of the free-energy on $\mathbf{F} = \mathbf{x}\nabla_0$, $\mathbf{P}$, n, p, θ, Eq. (1) yields :

$$\left[\rho\left(\frac{\partial\psi}{\partial\mathbf{F}} \cdot \mathbf{F}^T\right)^T - \boldsymbol{\sigma} + \mathbf{de} - \frac{\varepsilon_0}{2}(\mathbf{e} \cdot \mathbf{e})\mathbf{I} \right] \cdot\cdot(\dot{\mathbf{x}}\nabla) + \rho\left[\frac{\partial\psi}{\partial\mathbf{P}} - \mathbf{e}\right] \cdot \dot{\mathbf{P}} + \left[\frac{\partial\psi}{\partial n} - \mu_n\right]\rho\dot{n} + \left[\frac{\partial\psi}{\partial p} - \mu_p\right]\rho\dot{p}$$
$$+ \left[\eta + \frac{\partial\psi}{\partial\theta}\right]\rho\dot{\theta} + \nabla(\mu_n - q\varphi) \cdot \mathbf{j}_n + \nabla(\mu_p + q\varphi) \cdot \mathbf{j}_p + \frac{1}{\theta}\mathbf{q} \cdot (\nabla\theta) - (\mu_n + \mu_p)R \leq 0.$$

From classical considerations on different processes involving the independent variables, we have the following relations :

$$\boldsymbol{\sigma}(\mathbf{F}, \mathbf{P}, n, p, \theta) = \rho\left(\frac{\partial\psi}{\partial\mathbf{F}} \cdot \mathbf{F}^T\right)^T + \mathbf{de} - \frac{\varepsilon_0}{2}(\mathbf{e} \cdot \mathbf{e})\mathbf{I},$$

$$\mathbf{e}(\mathbf{F}, \mathbf{P}, n, p, \theta) = \frac{\partial\psi}{\partial\mathbf{P}},$$

$$\eta(\mathbf{F}, \mathbf{P}, n, p, \theta) = -\frac{\partial\psi}{\partial\theta}, \quad (2)$$

$$\mu_n(\mathbf{F}, \mathbf{P}, n, p, \theta) = \frac{\partial\psi}{\partial n}, \quad \mu_p(\mathbf{F}, \mathbf{P}, n, p, \theta) = \frac{\partial\psi}{\partial p},$$

and we are left with the reduced dissipation inequality

$$\nabla(\mu_n - q\varphi) \cdot \mathbf{j}_n + \nabla(\mu_p + q\varphi) \cdot \mathbf{j}_p + \frac{1}{\theta}\mathbf{q} \cdot (\nabla\theta) - (\mu_n + \mu_p)R \leq 0.$$

Ignoring possible cross couplings between the dissipative fluxes and the associated thermodynamic forces we assume the following linear relations

$$\mathbf{j}_n = -n\left(\frac{\rho}{q}\mathbf{M}_n\right) \cdot \nabla(\mu_n - q\varphi),$$

$$\mathbf{j}_p = -p\left(\frac{\rho}{q}\mathbf{M}_p\right) \cdot \nabla(\mu_p + q\varphi), \quad (3)$$

$$\mathbf{q} = -\mathbf{K} \cdot (\nabla\theta),$$

where $\mathbf{M}_n(\mathbf{F}, \mathbf{P}, \theta)$, $\mathbf{M}_p(\mathbf{F}, \mathbf{P}, \theta)$ and $\mathbf{K}(\mathbf{F}, \mathbf{P}, \theta)$ are positive-semidefinite rank 2 tensors of mobilities of electrons and holes, and conductivity respectively.

2.4 Consequences for a crystalline semiconductor

We now specify our model to crystalline semiconductor - such as silicon - which allows us to use the framework of small strains. Denoting by ε the small strain tensor, we use considerations of linear elasticity, linear electrostatic and statistical physics to give an explicit form to the free-energy function. The free-energy density is written as a sum of mechanical, electrostatic and electronic contributions

$$\widehat{\psi}(\varepsilon, \mathbf{P}, n, p) := \widehat{\psi}_{mech}(\varepsilon) + \widehat{\psi}_{elecs}(\mathbf{P}) + \widehat{\psi}_{elecn}(\varepsilon, n, p). \tag{4}$$

where

$$\widehat{\psi}_{mech}(\varepsilon) := \frac{1}{\rho}\left(\frac{\lambda}{2}(\mathrm{Tr}(\varepsilon))^2 + \mu \mathrm{Tr}(\varepsilon^2) \right),$$

where λ and μ are the Lamé coefficients of the material;

$$\widehat{\psi}_{elecs}(\mathbf{P}) := \frac{\rho}{2(\varepsilon_r - \varepsilon_0)}\mathbf{P}\cdot\mathbf{P}.$$

For the electronic part, denoting by $E_c(\varepsilon)$ and $E_v(\varepsilon)$ the band edge energy levels, $N_c(\varepsilon)$ and $N_v(\varepsilon)$ the effective densities of state of the conduction and valence bands respectively the associated free-energy density reads

$$\widehat{\psi}_{elecn}(\varepsilon, n, p) := n\left[k\theta\left(\ln\left(\frac{n}{N_c(\varepsilon)} \right) - 1 \right) + E_c(\varepsilon) \right] + p\left[k\theta\left(\ln\left(\frac{p}{N_v(\varepsilon)} \right) - 1 \right) - E_v(\varepsilon) \right],$$

where k is the Boltzman constant.

From the Helmholtz free energy density Eq. (4), we compute with Eqs. (2) the following constitutive relations

$$\sigma(\varepsilon, \mathbf{P}, n, p) = \underbrace{\lambda \mathrm{Tr}(\varepsilon)\mathbf{I} + 2\mu\varepsilon}_{\sigma_{mech}} + \underbrace{\rho n\left(-k\theta\frac{\partial \ln(N_c)}{\partial\varepsilon} + \frac{\partial E_c}{\partial\varepsilon} \right) + \rho p\left(-k\theta\frac{\partial \ln(N_v)}{\partial\varepsilon} - \frac{\partial E_v}{\partial\varepsilon} \right)}_{\sigma_{elecn}}$$

$$+ \underbrace{\rho\left(\mathbf{Pe} + \mathbf{eP} \right) + \varepsilon_0\left(\mathbf{ee} - \frac{1}{2}(\mathbf{e}\cdot\mathbf{e})\mathbf{I} \right)}_{\sigma_{maxw}}, \tag{5}$$

$$\mathbf{e}(\mathbf{P}) = \frac{\rho\mathbf{P}}{\varepsilon_r - \varepsilon_0},$$

$$\mu_n(\varepsilon, n) = E_c(\varepsilon) + k\theta\ln\left(\frac{n}{N_c(\varepsilon)} \right),$$

$$\mu_p(\varepsilon, p) = -E_v(\varepsilon) + k\theta\ln\left(\frac{p}{N_v(\varepsilon)} \right).$$

It is noteworthy in Eq. $(5)_1$ that the total stress tensor σ not only consists of a purely mechanical component (σ_{mech}) and a Maxwell component (σ_{maxw}) but contains also an electronic contribution (σ_{elecn}) which depends on electrons and holes densities; To the best of our knowledge, it is the first time this *electronic* contribution to the stress in semiconductors is brought out.

With Eqs. $(5)_{3,4}$ for the chemical potentials, we obtain from Eqs. (3) the drift-diffusion equations generalized to deformable media

$$\mathbf{j}_n = -k\theta\left(\frac{\rho}{q}\mathbf{M}_n(\varepsilon) \right)\cdot\nabla n + n\left(\frac{\rho}{q}\mathbf{M}_n(\varepsilon) \right)\cdot\left[q\nabla\varphi - \nabla E_c(\varepsilon) + k\theta\nabla\left(\ln(N_c(\varepsilon)) \right) \right],$$

$$\mathbf{j}_p = -k\theta\left(\frac{\rho}{q}\mathbf{M}_p(\varepsilon) \right)\cdot\nabla p + p\left(\frac{\rho}{q}\mathbf{M}_p(\varepsilon) \right)\cdot\left[-q\nabla\varphi + \nabla E_v(\varepsilon) + k\theta\nabla\left(\ln(N_v(\varepsilon)) \right) \right].$$

Considering in particular silicon, we compare, in order of magnitude, the relative sizes of the different components of the total stress tensor $(5)_1$. It appears that in the case of non-degenerate silicon the influence of electric field and electronic distribution on the stress is negligible, which reduces the couplings to the influence of strain on the electronic transport.

3 Bending of a *p-n* junction

In the present section, we make use of the governing field equations derived in Sec 2 to compute the current-voltage characteristic of a *p-n* junction subjected to non homogeneous strains as a result of the bending of the device.

We consider a *p-n* junction parallel to the mid-plane of a plate made of a crystalline semiconductor (see Fig. 1(a)), with Helmholtz free-energy given by Eq. (4). The junction occupies the space between
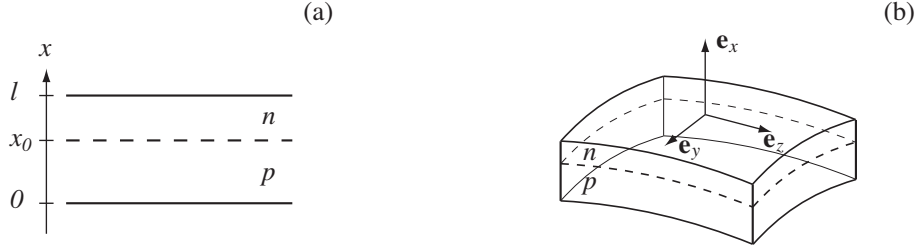

FIGURE 1 – In plane *p-n* junction. (a) Reference configuration $\mathcal{B}_0$, *n* and *p* denote the *n*-doped and *p*-doped regions respectively. (b) Deformed configuration bent about directions $\mathbf{e}_y$ and $\mathbf{e}_z$

the planes $x = 0$ and $x = l$ with *p-n* interface being the plane $x = x_0$.

3.1 Strain-induced changes in the electronic parameters

The plate is bent about the directions $\mathbf{e}_y$ and $\mathbf{e}_z$, so that the *yy*- and *zz*-components of the small-strain tensor, which determine the spatial variations of the electronic parameters, are given by

$$\varepsilon_{yy}(x,y,z) = \kappa_y(x-x_0) + \varepsilon_{yy}^0,$$
$$\varepsilon_{zz}(x,y,z) = \kappa_z(x-x_0) + \varepsilon_{zz}^0.$$

To model the strain-dependence of band energy levels, density of states and mobilities, we use linear relations derived from theoretical band structure computations and experimental measurements [8, 6, 12] :

$$E_c(\varepsilon) = E_c^r + \widetilde{\mathbf{E}}_c : \varepsilon, \qquad E_v(\varepsilon) = E_v^r + \widetilde{\mathbf{E}}_v : \varepsilon,$$
$$N_c(\varepsilon) = N_c^r + \widetilde{\mathbf{N}}_c : \varepsilon, \qquad N_v(\varepsilon) = N_v^r + \widetilde{\mathbf{N}}_v : \varepsilon,$$

where the superscript *r* denotes the value of the parameter in the relaxed state ($\varepsilon = \mathbf{0}$) and the rank-2 tensors $\widetilde{\mathbf{E}}_c$, $\widetilde{\mathbf{E}}_v$ and $\widetilde{\mathbf{N}}_c$, $\widetilde{\mathbf{N}}_v$ account for the first-order change of the corresponding quantities.

Similarly, the mobilities of electrons and holes are expressed as :

$$\mathbf{M}_n(\varepsilon) = \mathbf{M}_n^r + \widetilde{\mathbf{M}}_n : \varepsilon, \qquad \mathbf{M}_p(\varepsilon) = \mathbf{M}_p^r + \widetilde{\mathbf{M}}_p : \varepsilon,$$

where $\widetilde{\mathbf{M}}_n$ and $\widetilde{\mathbf{M}}_p$ are rank-4 tensors.

3.2 Governing equations of the electronic problem

The problem considered being one-dimensional along the *x*-direction, we reduce the general theory of Sec. 2 to 1D governing equations in terms of unknown fields $\{\varphi, n, p\}$

$$\begin{cases} \varepsilon_r \varphi'' = q\rho(n-p-C(x)), \\[2mm] j_n' = -R, \qquad j_n = -\dfrac{k\theta\rho}{q}m_n(x)n' + \dfrac{\rho}{q}m_n(x)n\big[q\varphi' - E_c(x)' + k\theta\big(\ln(N_c(x))\big)'\big], \\[2mm] j_p' = -R, \qquad j_p = -\dfrac{k\theta\rho}{q}m_p(x)p' + \dfrac{\rho}{q}m_p(x)p\big[-q\varphi' + E_v(x)' + k\theta\big(\ln(N_v(x))\big)'\big], \end{cases} \qquad (6)$$

where the recombination-generation R and intrinsic concentrations n_i are given by

$$R = \frac{\rho(pn - n_i^2(x))}{\tau_p(n + n_i(x)) + \tau_n(p + n_i(x))}, \qquad n_i^2(x) = N_c(x)N_v(x)\exp\left(\frac{-(E_c(x) - E_v(x))}{k\theta}\right).$$

The system of governing equations (6) is supplemented with the boundary conditions for $x = 0$ and $x = l$:

$$\begin{cases} n - p - C(x) = 0, \\ np = n_i(x)^2, \\ \varphi = \varphi_{bin} + \varphi_{app}. \end{cases}$$

3.3   Results

By means of asymptotic expansions with respect to the dimensionless curvature κ/l we compute, at first-order, the perturbation introduced by the strain on the fields $\{\varphi, n, p\}$. The resolution of the system (6) involves matched asymptotic expansions as a boundary layer develop at the p-n interface where the dopants concentration is discontinuous. Figure 2 shows the outer solution of system (6) where λ denotes the width of the boundary layer, L_n and L_p the diffusion lengths of electrons and holes respectively. The electrons and holes current combine to an electric current j constant throughout the device. The quantity
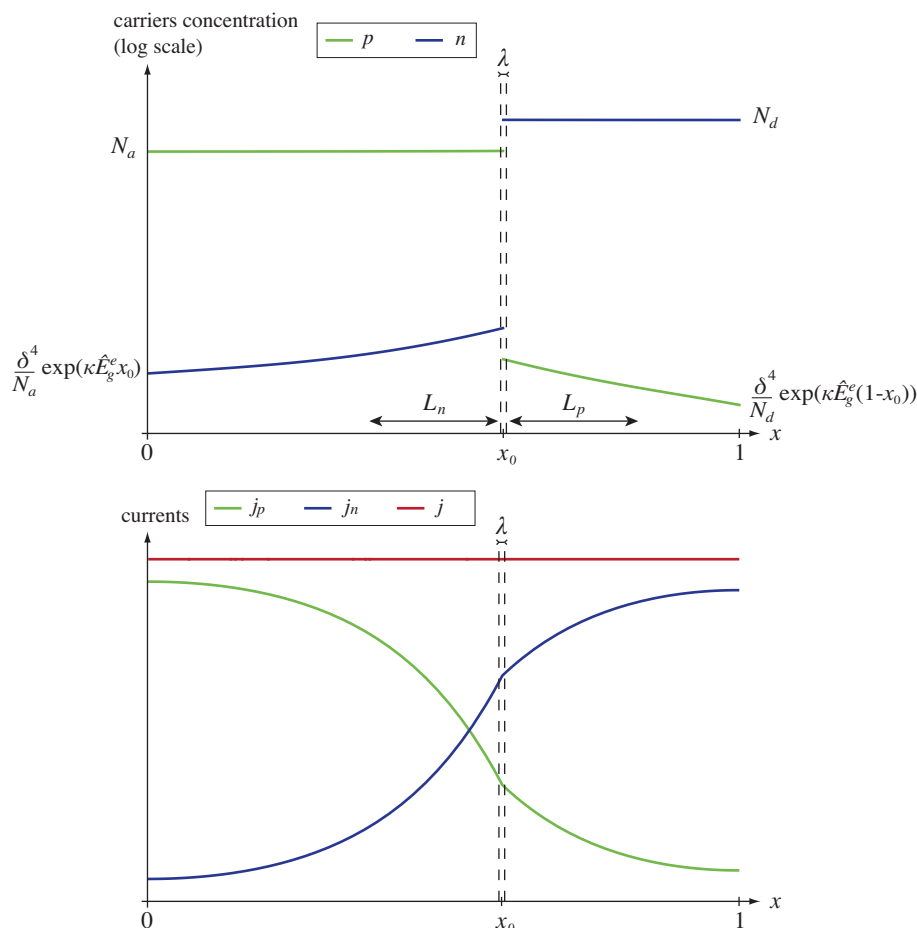

FIGURE 2 – Electrons and holes density and current distribution in the p-n junction.

of interest from a practical viewpoint is the current-voltage relation and how it is perturbed by strain. We obtain the usual Shockley relation for a p-n junction

$$j = \left[\exp(V) - 1\right] j_{sat},$$

where the saturation current j_{sat} is modified by the applied strain according to

$$j_{sat} = qU_T(\rho n_i^0)^2 \left(\frac{m_n^0}{(\rho N_a)L_n^0} \coth\left(\frac{x_0}{L_n^0}\right) + \frac{m_p^0}{(\rho N_d)L_p^0} \coth\left(\frac{l-x_0}{L_p^0}\right) \right.$$
$$+ \kappa \left\{ \frac{m_n^0}{(\rho N_a)} \left[\frac{\widehat{E}_g^e}{2kT} - \frac{\widehat{m}_n}{4m_n^0} \left(1 + \frac{x_0^2}{(L_n^0)^2 \sinh^2\left(\frac{x_0}{L_n^0}\right)} \right) \right] \right.$$
$$\left. \left. - \frac{m_p^0}{(\rho N_d)} \left[\frac{\widehat{E}_g^e}{2kT} - \frac{\widehat{m}_p}{4m_p^0} \left(1 + \frac{(l-x_0)^2}{(L_p^0)^2 \sinh^2\left(\frac{l-x_0}{L_p^0}\right)} \right) \right] \right\} \right).$$

The first order strain-induced change in the saturation current corresponds to the term that multiply the curvature κ.

3.4 Application to a monocrystalline silicon solar cell

Driven by the question of strain effect on the response of a solar cell, we apply the above results to compute the strain-induced change in the dark-current of a typical commercial solar cell made of a *p-n* junction.

Six different cases of strained solar cells are considered as depicted in Fig. 3.
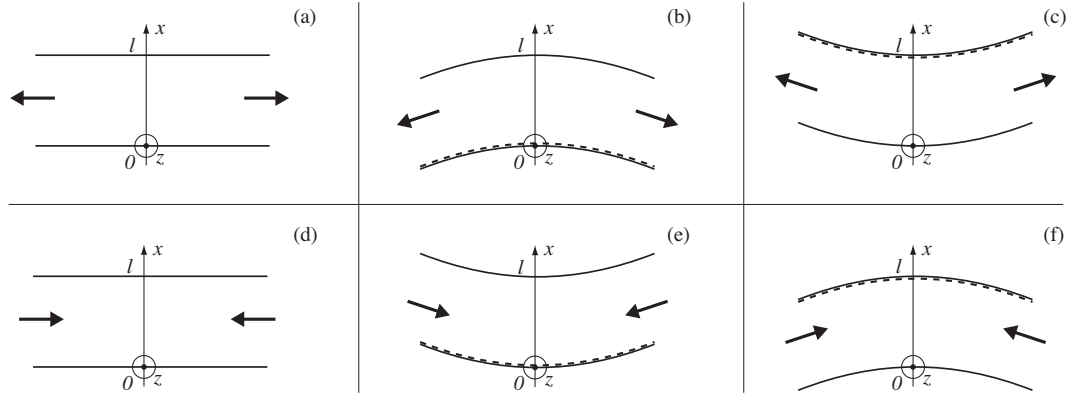

FIGURE 3 – Six strain states of the solar cell. (a) and (b) Homogeneous strain states while cases. (b), (c), (e) and (f), are non-homogeneous strain states due to the bending about *z*-axis. Regarding the *yy*-component of the strain, cases (a), (b), (c) are tensile state while cases (d), (e), (f), are compressive states. The dashed line indicates the neutral plane where $\varepsilon = \mathbf{0}$. For each case the maximum local value of ε_{xx} is 0.2 %.

The strain-induced changes in dark current $\Delta j = (j_{sat}(\varepsilon_{yy}^0, \kappa) - j_{sat}^r)/j_{sat}^r$ are summarized in Table 1 for the six strain states considered; they show a decrease (resp. increase) in dark current in tension (resp. compression) that can reach up to 24 %.

TABLE 1 – Strain-induced change in dark current for the six strain states depicted in Fig. 3

Case	(a)	(b)	(c)	(d)	(e)	(f)
Δj (%)	-19	-14	-4	24	19	6

4 Conclusion

In the present work, we address the strain effects in semiconductors using the framework of nonequilibrium thermodynamics, and subsequently apply the theory derived to a *p-n* junction device subjected to bending.

We find in the first part that, for crystalline semiconductors, the dominant interaction is the influence of strain on the electronic transport properties. As a result, the mechanical equilibrium can first be solved independently to compute the strain field that subsequently enters the electronic problem. However, the fully-coupled formulation shows the existence of an electronic contribution to the stress which, to the best of our knowledge, has not been mentioned in the literature.

In the second part of this work, we apply the general theory to compute the effect of bending on the current-voltage characteristic of a *p-n* junction. To this end, we solve the generalized drift-diffusion equations for a non-homogeneous linear strain field. By computing the characteristic of a *p-n* junction subject to bending. Finally, applying our result to the case of a monocrystalline silicon solar cell subjected to bending, we find that changes in dark current are up to 20 % for strains of 0.2 %. Finally, by comparing various uniform and nonuniform strain fields we find that the largest dark current changes are expected for the uniform strain loadings.

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