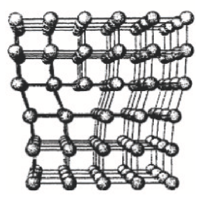
Weak discontinuity waves in n-type semiconductors with defects of dislocation

M. P. Mazzeo[a] and L. Restuccia[a]

[a]University of Messina, Department of Mathematical and Computer Sciences, Physical Sciences and Earth Sciences, Italy

Aim and motivation The propagation of weak discontinuities is investigated in an isotropic, homogenous and elastic *n*-type semiconductor with defects of dislocation. To this aim we introduce a new variable related to the surface across which the solutions or/and some of their derivatives undergo a jump. Following a Boillat's methodology for quasi-linear and hyperbolic systems of the first order, we obtain Bernoulli's equation governing the propagation of weak discontinuities.
Following A. Jeffrey in [2], the solution hypersurfaces of systems of PDEs are referred to as waves because they may be interpreted as representing propagating wavefronts. Some of the solutions present various types of discontinuities, when some surface is crossed, the solution or/and its derivatives undergo a jump. In this case it is said that the solution presents a ***shock***, or it is a ***shock wave*** or that we are in presence of a ***discontinuity waves*** (jumps of the first order derivatives) [1, 2].

Equation governing the evolution of electronic and dislocation fields We apply the theory developed in [3] for a semiconductor with defects of dislocation (see Fig.1) of *n*-type to a problem of a propagation of electronic-dislocation discontinuity waves in a *n*-type Ge.



Equations governing the electronic and dislocation fields evolution can reduce to the following form (see [3]):

$$\begin{cases} \rho\dot{n} + j^n_{k,k} = \frac{\rho n}{\tau^+} - \kappa a, \\ \tau^n \dot{j}^n_k - \alpha_n a_{,k} + \rho D_n n_{,k} = -j^n_k, \\ \dot{a} + \mathcal{V}_{k,k} = 0 \\ \tau^a \dot{\mathcal{V}}_k + D_a a_{,k} - \alpha_v n_{,k} = -\mathcal{V}_k. \end{cases}$$

where the superimposed dot denotes partial time derivative, the interaction between the electron and dislocation fluxes is disregarded and $\alpha_n = \alpha_n(a)$, $\alpha_v = \alpha_v(n)$ are coupling functions reflecting some new cross-kinetic effects during electronic-dislocation interactions. Furthermore, τ^+ denotes the life time of electrons, τ^n is the relaxation time of electrons, D_n and D_a are the diffusion coefficients on electrons and dislocations, respectively, τ^a denotes the relaxation time of dislocations, k is the recombination constant due to dislocations and the recombination function g^n has the form depending on the dislocation field. Moreover, we consider the relaxation semiconductor, so that $\tau^+ = \tau^n$, α_n and α_v are constant

One-dimensional case Now, we consider the one-dimensional case and we apply Boillat metodology for quasi-linear and hyperbolic systems of the first order, we obtain Bernoulli's equation governing the propagation of weak discontinuities. Assuming that the electronic-dislocation discontinuity wave propagation is along the x axis, the involved quantities depend on x_1, denoted by x, $x_2 = x_3 = 0$, we have:

$$\begin{cases} \frac{\partial n}{\partial t} + \frac{1}{\rho}\frac{\partial j^n_1}{\partial x} = \frac{n}{\tau^n} - \frac{\kappa a}{\rho}, \\ \frac{\partial j^n_1}{\partial t} - \frac{\alpha_n}{\tau^n}\frac{\partial a}{\partial x} + \frac{\rho D_n}{\tau^n}\frac{\partial n}{\partial x} = -\frac{j^n_1}{\tau^n}, \\ \frac{\partial j^n_2}{\partial t} = -\frac{j^n_2}{\tau^n}, \\ \frac{\partial j^n_3}{\partial t} = -\frac{j^n_3}{\tau^n}, \\ \frac{\partial a}{\partial t} + \frac{\partial \mathcal{V}_1}{\partial x} = 0 \\ \frac{\partial \mathcal{V}_1}{\partial t} + \frac{D_a}{\tau^a}\frac{\partial a}{\partial x} - \frac{\alpha_v}{\tau^a}\frac{\partial n}{\partial x} = -\frac{\mathcal{V}_1}{\tau^a}, \\ \frac{\partial \mathcal{V}_2}{\partial t} = -\frac{\mathcal{V}_2}{\tau^a}, \\ \frac{\partial \mathcal{V}_3}{\partial t} = -\frac{\mathcal{V}_3}{\tau^a}. \end{cases}$$

where $\alpha_n = \alpha_n(a)$ and $\alpha_v = \alpha_v(n)$. From the above system we have

$$j^n_2 = j^{n0}_2 e^{-\frac{1}{\tau^n}t} + f_1(x), \qquad j^n_3 = j^{n0}_3 e^{-\frac{1}{\tau^n}t} + f_2(x),$$

$$\mathcal{V}_2 = \mathcal{V}^0_2 e^{-\frac{1}{\tau^a}} + f_3(x), \qquad \mathcal{V}_3 = \mathcal{V}^0_3 e^{-\frac{1}{\tau^a}} + f_4(x).$$

Then, the remained system reads

$$\mathbf{U}_t + \mathbf{A}(\mathbf{U})\mathbf{U}_x = \mathbf{B}(\mathbf{U})$$

where $\mathbf{U} = (n, j^n_1, a, \mathcal{V}_1)^T$, and

$$\mathbf{B} = \left(\frac{n}{\tau^+} - \frac{\kappa a}{\rho}, -\frac{j^n_1}{\tau^n}, 0, -\frac{\mathcal{V}_1}{\tau^a},\right)^T$$

and

$$\mathbf{A} = \begin{pmatrix} 0 & \frac{1}{\rho} & 0 & 0 \\ \frac{\rho D_n}{\tau^n} & 0 & -\frac{\alpha_n}{\tau^n} & 0 \\ 0 & 0 & 0 & 1 \\ -\frac{\alpha_v}{\tau^a} & 0 & \frac{D_a}{\tau^a} & 0 \end{pmatrix},$$

In our case, being $\mathbf{n} = (n_1, 0, 0)$, $\mathbf{A}_n(\mathbf{U}) = \mathbf{A}n_1$ having the form

$$\mathbf{A}n_1 = \begin{pmatrix} 0 & \frac{1}{\rho}n_1 & 0 & 0 \\ \frac{\rho D_n}{\tau^n}n_1 & 0 & -\frac{\alpha_n}{\tau^n}n_1 & 0 \\ 0 & 0 & 0 & n_1 \\ -\frac{\alpha_v}{\tau^a}n_1 & 0 & \frac{D_a}{\tau^a}n_1 & 0 \end{pmatrix}$$

The matrix $\mathbf{A}n_1$ admits the following simple eigenvalues:

$$\lambda^{(\pm)}_1 = \pm\frac{1}{\sqrt{2}}\sqrt{\frac{\rho D_n\tau^a + \rho D_a\tau^n - G}{\rho\tau^n\tau^a}},$$

$$\lambda^{(\pm)}_2 = \pm\frac{1}{\sqrt{2}}\sqrt{\frac{\rho D_n\tau^a + \rho D_a\tau^n + G}{\rho\tau^n\tau^a}},$$

$$G = \sqrt{(\rho D_n\tau^a - \rho D_a\tau^n)^2 + 4\rho\alpha_n\alpha_v\tau^n\tau^a}.$$

The eigenvalues $\lambda^{(\pm)}_1$ are real when the condition $\rho D_n\tau^a + \rho D_a\tau^n - G \geq 0$ is valid, i.e. $\alpha_n\alpha_v \leq D_n D_a$. The eigenvalues $\lambda^{(\pm)}_2$ are always real. The left eigenvectors $\mathbf{l}^{(\pm)}_1$, $\mathbf{l}^{(\pm)}_2$, and the right eigenvectors $\mathbf{r}^{(\pm)}_1$, $\mathbf{r}^{(\pm)}_2$ corresponding, to eigenvalues $\lambda^{(\pm)}_1$, $\lambda^{(\pm)}_2$, have the form

$$\mathbf{l}^{(\pm)}_1 = \left(\frac{\rho}{n_1}\lambda^{(\pm)}_1, 1, \frac{\lambda^{(\pm)}_1\mathcal{S}}{2n_1\alpha_v\tau^n}, \frac{\mathcal{S}}{2\alpha_v\tau^n}\right),$$

$$\mathbf{l}^{(\pm)}_2 = \left(\frac{\rho}{n_1}\lambda^{(\pm)}_2, 1, -\frac{\lambda^{(\pm)}_2\mathcal{R}}{2n_1\alpha_v\tau^n}, -\frac{\mathcal{R}}{2\alpha_v\tau^n}\right),$$

$$\mathbf{r}^{(\pm)}_1 = \left(\frac{\tau^n\lambda^{(\pm)}_1\mathcal{R}}{\rho n_1\mathcal{C}}, 1, \frac{2\alpha_v(\tau^n)^2\lambda^{(\pm)}_1}{n_1\mathcal{C}}, \frac{2\alpha_v(\tau^n)^2\left(\lambda^{(\pm)}_1\right)^2}{\mathcal{C}}\right),$$

$$\mathbf{r}^{(\pm)}_2 = \left(-\frac{\tau^n\lambda^{(\pm)}_2\mathcal{S}}{\rho n_1\mathcal{L}}, 1, \frac{2\alpha_v(\tau^n)^2\lambda^{(\pm)}_2}{n_1\mathcal{L}}, \frac{2\alpha_v(\tau^n)^2\left(\lambda^{(\pm)}_2\right)^2}{\mathcal{L}}\right),$$

with

$$\mathcal{R} = (-\rho D_n\tau^a + \rho D_a\tau^n + G) \qquad \mathcal{S} = (\rho D_n\tau^a - \rho D_a\tau^n + G)$$

$$\mathcal{C} = (-1)\left[\rho D^2_n\tau^a + 2\alpha_v\alpha_n\tau^n - D_n(\rho D_a\tau^n + G)\right]$$

$$\mathcal{L} = (-1)\left[\rho D^2_n\tau^a + 2\alpha_v\alpha_n\tau^n - D_n(\rho D_a\tau^n - G)\right]$$

They are linearly independent, so the system $\mathbf{U}_t + \mathbf{A}(\mathbf{U})\mathbf{U}_x = \mathbf{B}(\mathbf{U})$ is hyperbolic. The discontinuity waves which are propagating with the velocity given by $\lambda^{(\pm)}_1$ and $\lambda^{(\pm)}_2$ are not exceptional waves in the sense of Lax-Boillat [1], because

$$\nabla\lambda^{(\pm)}_1 \cdot \mathbf{r}^{(\pm)}_1 = \frac{-\alpha_n\tau^n\mathcal{R}\frac{\partial\alpha_v}{\partial n} - 2\rho(\alpha_v\tau^n)^2\frac{\partial\alpha_n}{\partial a}}{2\rho n_1 G\mathcal{C}} \neq 0$$

$$\nabla\lambda^{(\pm)}_2 \cdot \mathbf{r}^{(\pm)}_2 = \frac{-\alpha_n\tau^n\mathcal{S}\frac{\partial\alpha_v}{\partial n} + 2\rho(\alpha_v\tau^n)^2\frac{\partial\alpha_n}{\partial a}}{2\rho n_1 G\mathcal{L}} \neq 0,$$

with

$$\nabla \equiv \left(\frac{\partial}{\partial n}, \frac{\partial}{\partial j^n_1}, \frac{\partial}{\partial a}, \frac{\partial}{\partial\mathcal{V}_1},\right).$$

We fix our attention on $\lambda = \lambda^{(+)}_2$, which corresponds to a progressive fast wave traveling to the right. Analogous results are valid for the waves propagating with the other velocities.
The eigenvectors left and right $\mathbf{l} = \mathbf{l}^{(+)}_2$ and $\mathbf{r} = \mathbf{r}^{(+)}_2$, corresponding to $\lambda^{(+)}_2$ satisfy the following relation

$$\mathbf{l}^{(+)}_2 \cdot \mathbf{r}^{(+)}_2 = \frac{\tau^n\left(\frac{1}{\sqrt{2}}\sqrt{\frac{\rho D_n\tau^a + \rho D_a\tau^n + G}{\rho\tau^n\tau^a}}\right)^2(3\rho D_n\tau^a - 3D_a\tau^n - G)}{\mathcal{L}} + 1.$$

The characteristic rays are

$$\frac{dt}{d\sigma} = 1 \qquad \frac{dx_i}{d\sigma} = \frac{\partial\Psi^0}{\partial\Phi_\alpha} = \left(\lambda^{(+)}_2\right)_0, \qquad \frac{d\Phi_\alpha}{d\sigma} = 0,$$

Now, we consider an uniform unperturbed state in which $\mathbf{U}^0$, solution of the system $\mathbf{U}_t + \mathbf{A}(\mathbf{U})\mathbf{U}_x = \mathbf{B}(\mathbf{U})$, has the form $\mathbf{U}^0 = (n^0, 0, a^0, 0)$, with n^0 and a^0 constants. In $\mathbf{U}^0$ we have

$$\left(\lambda^{(+)}_2\right)_0 = \frac{1}{\sqrt{2}}\sqrt{\frac{\rho^0 D_n\tau^a + \rho^0 D_a\tau^n + G^0}{\rho^0\tau^n\tau^a}},$$

$$\left(\mathbf{l}^{(+)}_2\right)_0 = \left(\frac{\rho^0}{n^0_1}\left(\lambda^{(+)}_2\right)_0, 1, -\frac{\left(\lambda^{(+)}_2\right)_0\mathcal{R}^0}{2n^0_1\alpha^0_v\tau^n}, -\frac{\mathcal{R}^0}{2\alpha^0_v\tau^n}\right),$$

$$\left(\mathbf{r}^{(+)}_2\right)_0 = \left(-\frac{\tau^n\left(\lambda^{(+)}_2\right)_0\mathcal{S}^0}{\rho^0 n^0_1\mathcal{L}^0}, 1, \frac{2\alpha_v(\tau^n)^2\left(\lambda^{(+)}_2\right)_0}{n^0_1\mathcal{L}^0}, \frac{2\alpha_v(\tau^n)^2\left[\left(\lambda^{(+)}_2\right)_0\right]^2}{\mathcal{L}^0}\right),$$

$$\left(\mathbf{l}^{(+)}_2 \cdot \mathbf{r}^{(+)}_2\right)_0 = \frac{\tau^n\left[\left(\lambda^{(+)}_2\right)_0\right]^2(3\rho^0 D_n\tau^a - 3D_a\tau^n - G^0)}{\mathcal{L}^0} + 1$$

and

$$\left(\nabla\lambda^{(+)}_2 \cdot \mathbf{r}^{(+)}_2\right)_0 = \frac{-\alpha^0_n\tau^n\mathcal{S}^0\left(\frac{\partial\alpha_v}{\partial n}\right)^0 + 2\rho^0(\alpha^0_v\tau^n)^2\left(\frac{\partial\alpha_n}{\partial a}\right)^0}{2\rho^0 n^0_1 G^0\mathcal{L}^0},$$

where the symbol " ^{0} " indicates that the quantities are calculated in U^0. The radial velocity along the characteristic rays is

$$\mathbf{\Lambda}^0(\mathbf{U}^0, \mathbf{n}^0) = \left(\lambda^{(+)}_2\right)_0\mathbf{n}^0 = \frac{1}{\sqrt{2}}\sqrt{\frac{\rho_0 D_n\tau^a + \rho_0 D_a\tau^n + G_0}{\rho_0\tau^n\tau^a}}\,\mathbf{n}^0.$$

By integration of the characteristic rays one obtain

$$x^0 = \sigma = t, \qquad x = (x)^0 + \lambda^{(+)}_2(\mathbf{U}^0)\sigma = (x)^0 + \gamma^0 t,$$

and the wave front in the first approximation is

$$\varphi(t, x) = \varphi^0\left(x(t) - \gamma^0 t\right),$$

where

$$\gamma^0 = \gamma(\mathbf{U}^0) = \left(\lambda^{(+)}_2\right)_0 = \frac{1}{\sqrt{2}}\sqrt{\frac{\rho_0 D_n\tau^a + \rho_0 D_a\tau^n + G_0}{\rho_0\tau^n\tau^a}}.$$

The amplitude $\pi(x, t)$ satisfies the following equation:

$$\left(\mathbf{l}^{(+)}_2 \cdot \mathbf{r}^{(+)}_2\right)_0\left\{\frac{d\pi}{d\sigma} + (|\varphi_x|)_0\left(\nabla\lambda^{(+)}_2 \cdot \mathbf{r}^{(+)}_2\right)_0\pi^2\right\} = c^0\,\pi,$$

where

$$c^0 = \left[\nabla\left(\mathbf{l}^{(+)}_2 \cdot \mathbf{B}\right) \cdot \mathbf{r}^{(+)}_2\right]_0$$

Taking into account that

$$\mathbf{l}^{(+)}_2 \cdot \mathbf{B} = \frac{\rho\lambda^{(+)}_2}{n_1}\left(\frac{n}{\tau^n} - \frac{\kappa a}{\rho}\right) - \frac{j^n_1}{\tau^n} + \frac{\mathcal{V}_1\mathcal{R}}{2\alpha_v\tau^n\tau^a},$$

$$\nabla\left(\mathbf{l}^{(+)}_2 \cdot \mathbf{B}\right) = \left(\frac{\partial\left(\mathbf{l}^{(+)}_2 \cdot \mathbf{B}\right)}{\partial n}, \frac{\partial\left(\mathbf{l}^{(+)}_2 \cdot \mathbf{B}\right)}{\partial j}, \frac{\partial\left(\mathbf{l}^{(+)}_2 \cdot \mathbf{B}\right)}{\partial a}, \frac{\partial\left(\mathbf{l}^{(+)}_2 \cdot \mathbf{B}\right)}{\partial\mathcal{V}}\right),$$

where

$$\frac{\partial\left(\mathbf{l}^{(+)}_2 \cdot \mathbf{B}\right)}{\partial n} = \frac{\rho\alpha_n}{G}\frac{\partial\alpha_v}{\partial n}\left[\frac{1}{2\lambda^{(+)}_2 n_1}\left(\frac{n}{\tau^n} - \frac{\kappa a}{\rho}\right) + \frac{\mathcal{V}_1}{\alpha_v}\right] + \frac{\rho\lambda}{n_1\tau^n} + \frac{\mathcal{V}_1\mathcal{R}}{2\alpha^2_v\tau^n\tau^a}\frac{\partial\alpha_v}{\partial n},$$

$$\frac{\partial\left(\mathbf{l}^{(+)}_2 \cdot \mathbf{B}\right)}{\partial j} = -\frac{1}{\tau^n},$$

$$\frac{\partial\left(\mathbf{l}^{(+)}_2 \cdot \mathbf{B}\right)}{\partial a} = \frac{\rho\alpha_v}{2n_1\lambda^{(+)}_2 G}\frac{\partial\alpha_n}{\partial a}\left(\frac{n}{\tau^n} - \frac{\kappa a}{\rho}\right) - \lambda^{(+)}_2\frac{\kappa}{n_1} + \frac{\rho\mathcal{V}_1}{G}\frac{\partial\alpha_n}{\partial a},$$

$$\frac{\partial\left(\mathbf{l}^{(+)}_2 \cdot \mathbf{B}\right)}{\partial\mathcal{V}} = \frac{\mathcal{R}}{2\alpha_v\tau^n\tau^a}.$$

From the above results we obtain

$$h(\sigma) = \pi^0 exp\left[-\int_0^\sigma \frac{c^0}{\left(\mathbf{l}^{(+)}_2 \cdot \mathbf{r}^{(+)}_2\right)_0}d\tau\right], \quad \Phi(\sigma) = 1 + \int_0^\sigma \left(\nabla\lambda^{(+)}_2 \cdot \mathbf{r}^{(+)}_2\right)_0 hd$$

Relation above gives

$$\Phi(\sigma) = 1 + \int_0^\sigma \frac{h}{2\rho^0 n^0_1 G^0\mathcal{L}^0}\left[-\alpha^0_n\tau^n\mathcal{S}^0\left(\frac{\partial\alpha_v}{\partial n}\right)^0 + 2\rho^0(\alpha^0_v\tau^n)^2\left(\frac{\partial\alpha_n}{\partial a}\right)^0\right]d\tau.$$

In the case in which there exists a critical time σ_c where $\Phi(\sigma_c) = 0$, then $\pi \to \infty$, and this may correspond to a shock wave [1].

References

[1] **Boillat, G.**, La propagation des ondes, Gauthier-Villars, Paris, 1965.

[2] **Jeffrey, A.**, Quasilinear hyperbolic systems and waves, Pitman, London, 1976.

[3] **L.Restuccia and B.Maruszewski**, "Interactions between electronic field and dislocations in a deformable semiconductor", *Int. Journal of Applied Electromagnetics and Mechanics*, **6**, 139-153 (1995).

[4] **M.P. Mazzeo, L. Restuccia**, "Thermodynamics of extrinsic semiconductors with dislocations", *Communication to SIMAI Congress*, ISSN: 1827-9015, DOI: 10.1685/CSC06113, ISSN: 1970-4429 (2006).