Dislocation dynamics described by non-local Hamilton-Jacobi equations

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Abstract

We study a mathematical model describing dislocation dynamics in crystals. This phase-field model is based on the introduction of a core tensor which mollifies the singular field on the core of the dislocation. We present this model in the case of the motion of a single dislocation, without cross-slip. The dynamics of a single dislocation line, moving in its slip plane, is described by an Hamilton-Jacobi equation whose velocity is a non-local quantity depending on the whole shape of the dislocation line. Introducing a level sets formulation of this equation, we prove the existence and uniqueness of a continuous viscosity solution when the dislocation stays a graph in one direction. We also propose a numerical scheme for which we prove that the numerical solution converges to the continuous solution.

Key words: Dislocation dynamics, Peach-Koehler force, Hamilton-Jacobi equations, viscosity solutions, level sets method, non-local equations.
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1. Introduction

Since the beginning of the 90's, a lot of work has been done to develop Discrete Dislocation Dynamics (see for instance [1] to only cite one work). Recently, a new approach, called the *phase field model of dislocations* has emerged, where dislocations are described by the variation of continuous fields (see Rodney, Le Bouar and Finel [2], Xiang, Cheng, Srolovitz, E [3], Wang, Jin, Cuitino, Khachaturyan [4], Cuitino, Koslowski, Ortiz [5]). In this approach, possible topological changes during the dislocation movement are automatically taken into account by the model. In the present paper, we study the phase field model of dislocation dynamics which has been recently proposed by Rodney, Le Bouar and Finel [2], and propose a general presentation based on the notion of core

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tensor.

2. The general model

Let us consider an orthonormal basis (e_1, e_2, e_3) of $\mathbb{R}^3$. In this section we denote the coordinates by $x = (x_1, x_2, x_3)$, and $x' = (x_1, x_2)$.

2.1. *Dislocation dynamics for a single dislocation*

Let us assume that the dislocation line is represented by the boundary Γ of a smooth bounded domain $\Omega \subset \mathbb{R}^2$. We define $\rho(x')$ the characteristic function of Ω, which is equal to 1 if $x' \in \Omega$ and zero if $x' \in \mathbb{R}^2 \backslash \Omega$.
Let us call $n = e_3$ the normal to the slip plane, and b the Burgers vector. We set $\varepsilon^0_{ij} = \frac{1}{2}(b_i n_j + b_j n_i)$. The plane $\mathbb{R}^2$ is assumed to be the plane where the dislocation can move. This plane is naturally imbedded in the three-dimensional material which is assumed to be the whole space $\mathbb{R}^3$.

The classical theory of dislocations asserts that the dislocation line Γ creates a distorsion in the classical strain ε^{cl} such that

$$\varepsilon^{cl}_{ij} = \rho \delta_0(x_3) \varepsilon^0_{ij} + \varepsilon_{ij}(U)$$

where $\delta_0(x_3)$ is the Dirac mass only in the x_3 component and $U(x) = U = (U_1, U_2, U_3)$ is a displacement which defines $\varepsilon_{ij}(U) = \frac{1}{2}(U_{i,j} + U_{j,i})$.
Here the energy formally associated to this strain is $\int_{\mathbb{R}^3} \frac{1}{2} \Lambda_{ijkl} \varepsilon^{cl}_{ij} \varepsilon^{cl}_{kl}$ where Λ_{ijkl} are the coefficients of elasticity. Minimizing on U, we find that the strain ε^{cl}_{ij} is given by $\varepsilon^{cl}_{ij} = R_{ijkl} \varepsilon^0_{kl} \star \rho \delta_0(x_3)$, where R_{ijkl} is a kind of Green function. The difficulty in this approach is that the energy is infinite because the strain field ε^{cl} is too singular on the dislocation line itself. To overcome this difficulty, we propose to introduce a core tensor χ_{ijkl} which satisfies $\int_{\mathbb{R}^3} \chi_{ijkl} = \frac{1}{2}(\delta_{ij}\delta_{kl} + \delta_{jk}\delta_{il})$ and the symmetry conditions $\chi_{ijkl} = \chi_{klij} = \chi_{jikl}$. This core tensor will describe the fine structure of the core of the dislocation. Then the “true physical strain” is given by the convolution

$$\varepsilon_{ij} = \chi_{ijkl} \star \left(\rho \delta_0(x_3) \varepsilon^0_{ij}\right) + \varepsilon_{ij}(U) \ .$$

Now the energy of the line is well defined

$$E(\Gamma) = \int_{\mathbb{R}^3} \frac{1}{2} \Lambda_{ijkl} \varepsilon_{ij} \varepsilon_{kl}$$

if χ_{ijkl} is smooth enough, and the displacement U is chosen to minimize this energy, i.e. satisfying the following equations of elasticity

$$\left(\Lambda_{ijkl}\ \varepsilon_{kl}\right)_{,i} = 0 \ .$$

A typical choice which matches with the Peierls-Nabarro model for isotropic elasticity is $\chi_{ijkl} = \chi_0(x_1, x_2)\delta_0(x_3)\frac{1}{2}(\delta_{ij}\delta_{kl} + \delta_{jk}\delta_{il})$ where the Fourier transform of χ_0 is $\hat{\chi}_0(\xi_1, \xi_2) = -\frac{\mu b^2}{2}\left(\frac{\xi_1^2 + \frac{1}{1-\nu}\xi_2^2}{\sqrt{\xi_1^2+\xi_2^2}}\right) e^{-\frac{\zeta}{2}\sqrt{\xi_1^2+\xi_2^2}}$ with $\zeta > 0$ a parameter proportional to the size of the core of the dislocation, ν the Poisson ratio, μ a Lamé coefficient, and $b = |b| e_1$.
To evaluate the resolved Peach-Koehler force acting on the dislocation line, we can proceed as follows. We denote by $n_\Gamma(s)$ the outer unit normal to Ω, contained in the slip plane and parametrized by the curvilinear abscissa s of Γ. For a given $\delta > 0$, we consider a variation of Γ defined by $\Gamma_\delta(s) = \Gamma(s) + \delta h(s) n_\Gamma(s)$ for any general function h. Then a computation gives

$$-\frac{d}{d\delta} E(\Gamma_\delta)_{|\delta=0} = \int_\Gamma ds\ h(s) c(\Gamma(s)) \qquad (1)$$

where the function

$$c = c_0 \star \rho$$

is called the generalized resolved Peach-Koehler force, and $c_0(x') = \left(\check{R}_{klmn} \star \check{\chi}_{mnpq} \varepsilon^0_{pq} \star \Lambda_{ijkl} R_{ijab} \star \chi_{abcd} \varepsilon^0_{cd}\right)(x', 0)$ where $\check{f}(x) = f(-x)$ for any general function f. Classically dislocation dynamics of $\Gamma = \Gamma_t$ is defined by

$$\frac{d\Gamma_t}{dt}(s) = \frac{1}{B}\ c(\Gamma_t(s)) n_{\Gamma_t}(s)$$

where B is a viscous drag coefficient. To simplify the presentation we assume from now on that $B = 1$. Then this equation is equivalent to a single non-local equation satisfied by $\rho(x', t)$, namely

$$\frac{\partial \rho}{\partial t} = (c_0 \star \rho)\, |\nabla \rho| \ . \qquad (2)$$

This non-local Hamilton-Jacobi equation describes the self-dynamics of a single dislocation line and is studied in details in [6,7].

2.2. *Dislocation dynamics for several dislocations*

In this subsection we consider the case of N dislocations $\Gamma^\alpha,\ \alpha = 1, ..., N$, which are the boundaries of open sets Ω^α contained in the planes defined by $\{x \cdot n^\alpha = a^\alpha\}$, with burgers vectors b^α. We define $\varepsilon^{0\alpha}_{ij} = \frac{1}{2}\left(b^\alpha_i n^\alpha_j + b^\alpha_j n^\alpha_i\right)$. We set ρ^α the characteristic functions of Ω^α. Then

$$\varepsilon_{ij} = \sum_\alpha \chi^\alpha_{ijkl} \star \left(\rho^\alpha \delta_0(x \cdot n^\alpha - a^\alpha)\varepsilon^{0\alpha}_{ij}\right) + \varepsilon_{ij}(U)$$

and the energy is

$$E(\Gamma^1, ..., \Gamma^N) = \int_{\mathbb{R}^3} \frac{1}{2}\Lambda_{ijkl}\varepsilon_{ij}\varepsilon_{kl} + \sigma^{ext}_{ij}\varepsilon_{ij}$$

if σ^{ext}_{ij} is an exterior applied stress. Finally the resolved Peach-Koehler force c^α can be computed still using formula (1), and the functions ρ^α satisfy the Hamilton-Jacobi equations $\dfrac{\partial \rho^\alpha}{\partial t} = c^\alpha\, |\nabla \rho^\alpha|$.

3. The level sets formulation for a single dislocation

In equation (2), the function ρ is discontinuous. It is more convenient to localize the dislocation as the zero level set of a function $u(x_1, x_2, t)$, i.e. $\Gamma_t = \left\{x' \in \mathbb{R}^2,\ u(x', t) = 0\right\}$ where u solves the following equation

$$\begin{cases} \dfrac{\partial u}{\partial t} = (c_0 \star [u])\,|\nabla u| \\ u(x', 0) = u^0(x') \end{cases} \qquad (3)$$

with $[u] = 1$ if $u > 0$ and $[u] = 0$ if $u \le 0$, and u^0 is the initial condition. The solution of this equation should be understood in the viscosity sense, see [9] for a general theory.
For this equation we have the following result

Theorem 1 (Short time existence and uniqueness)
Let u^0 satisfying $|\nabla u^0(x')| < B$ in $\mathbb{R}^2$ and $\dfrac{\partial u^0}{\partial x_2}(x') > b > 0$ in $\mathbb{R}^2$. Let c_0 be such that $|c_0(x')|, |\nabla c_0(x')| \le \dfrac{C}{(1 + |x'|^2)^{\frac{3}{2}}}$. Then there exists $T^* > 0$ such that there exists a unique (viscosity) solution u of (3) on $\mathbb{R}^2 \times [0, T^*)$.

The proof of this result is done in a work in preparation.

4. A numerical scheme

We build a first order finite difference scheme, essentially using a monotone numerical Hamiltonian for the norm of the spatial gradient, discrete convolution for the non local speed and forward Euler for the time derivative.

Given a lattice $Q_d = \{(I\Delta x, n\Delta t) : I, n \in \mathbb{Z}^2 \times \mathbb{N}\}$, we will denote with (x'_I, t_n) the node $(i\Delta x, j\Delta x, n\Delta t)$ with $I = (i, j)$, and with $v^n = (v^n_I)_I$ the values of the numerical approximation of the exact solution $u(x'_I, t_n)$.

The main difficulty is clearly due to the non local term, that requires the availability of the solution we are intending to approximate. To circumvent this problem, we *freeze* the solution at each time step $[t_n, t_{n+1}]$ and we apply a monotone scheme S^n for local Hamilton Jacobi equation, with a smaller time scale $\Delta\tau = \Delta t^3$:

$$\Delta\tau = \frac{\Delta t}{M},\ \tau^n_m = t_n + m\Delta\tau,\ m = 0, ..., M\ .$$

Given the intial condition $v^0_I = u^0(x'_I)$, we solve

$$\begin{cases} w^{n,0}_I = v^n_I \\ w^{n,m+1}_I = S^n(w^{n,m}, I) \quad m = 0, ..., M-1 \end{cases} \qquad (4)$$

then we update the discrete convolution each time step $\Delta t = M\Delta\tau$:

$$v^{n+1}_I = w^{n,M}_I \quad n = 0, ..., N.$$

The S^n schemes, depending on v^n, are explicit marching schemes:

$$S^n(w^{n,m}, I) = w^{n,m}_I + \Delta\tau H_d([v^n], Dw^{n,m}_I, I)$$

where $Dw^{n,m}_I = \left(D^\pm_{x_1} w^{n,m}_I, D^\pm_{x_2} w^{n,m}_I\right)$ are the standard forward and backward first difference.

Here H_d is a discrete numerical Hamiltonian, depending on the discrete convolution

$$c_I([v^n]) = \sum_{J\in\mathbb{Z}^2} c^0_{I-J}[v^n]_J \Delta x_1 \Delta x_2,$$

where $[v^n]_J = 1$ if $v^n_J > 0$ and $[v^n]_J = 0$ if $v^n_J \leq 0$. The discrete numerical Hamiltonian is a numerical monotone Hamiltonian, for instance the one proposed by Osher and Sethian in [8]. For this scheme, we prove the

Theorem 2 (Numerical error estimate)
Under the assumptions of theorem 1, let us consider the solution u defined on $\mathbb{R}^2 \times [0, T^*)$. Let $w^{n,m}_I$ be the solution of the scheme (4), that is monotone under certain CFL condition. Then there exists a constant $C > 0$ such that for $n = 0, ...N$, $m = 0, ..., M-1$:

$$\sup_{I\in\mathbb{Z}^2} |u(x'_I, n\Delta t + m\Delta\tau) - w^{n,m}_I| \leq C\,(\Delta\tau)^{\frac{1}{3}}$$

5. Conclusions

The main result of our work is to propose a mathematical formulation of a phase field model of dislocation dynamics. We think that this is an important first step because the model can now be studied by the community of mathematicians. We hope that this will have consequences both on the modelling of dislocation dynamics and on numerical methods to compute dislocation dynamics.

In our model, the position of a dislocation loop in its glide plane is described by a discontinuous field ρ which is equal to 1 inside the loop and 0 outside. In order to obtain the mechanical state within the framework of linear elasticity, we introduce a "core tensor" to remove the unphysical divergences near the dislocation core. Then, assuming that the local speed of the dislocation is proportional to the resolved Peach and Khoeler force, we derive the kinetic equation for the dislocation field ρ.

This equation falls into the general class of non local Hamilton Jacobi equations. At this point, a mathematical difficulty arises, because the kinetic equation may admit several solutions. To avoid this problem, we have used the concept of viscosity solutions (see [9]) which helps to choose the physical solution.

A great benefit of the present mathematical formulation is the development and adaptation of well controled numerical algorithms. In the present work, we have shown how to use the Level Set method in the simplified case of a single dislocation line. Compared to the algorithm used in [2], our scheme does not introduce numerical anisotropy, and we have obtained an exact result for the numerical error.

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