A Model of the Evolution of a Two-dimensional Defective Structure *

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Abstract. A model of the anelastic evolution law of a two-dimensional defective solid crystal body is proposed. Assuming that the material body is made of triclinic crystals and that the evolution process does not alter the basic material symmetry group we postulate that the evolution is driven by the present state of the density of the distribution of defects. We show that a linear relation between the inhomogeneity velocity gradient and the torsion tensor is rich enough to model such phenomena as relaxation of defects and dislocation pile-up.

Keywords: defects, evolution, inhomogeneity, anelasticity

1. Introduction

The theory of continuous distributions of dislocations in its various formulations results always in a mathematical description of distributions of inhomogeneities in terms of differential-geometric objects. An open question, however, is the formulation of constitutive laws that govern the possible time evolution of such geometric structures so as to represent a variety of important physical phenomena involving the massive motion of defects. The driving force behind these phenomena can perhaps be best explained in terms of configurational forces such as those represented by the Eshelby tensor. Nevertheless, it is quite possible to conceive of an evolutionary process that is driven by the dislocation pattern itself in its natural tendency to eliminate residual stresses or, even if these stresses are absent, to achieve a defect-free structure over time. These processes can be enhanced, for example, by raising the temperature of the body so as to increase the probability of the atoms in overcoming potential barriers. On the other hand, a dislocation pattern may lead in the opposite direction, in the sense that a dislocation pile-up may arise naturally out of an initially smooth distribution of defects. These typically nonlinear phenomena are in

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need of a general theoretical framework consistent with the differential-geometric apparatus mentioned above. The purpose of this paper is to show how a relatively simple model, valid for solids endowed with only a discrete material symmetry group and already possibly devoid of residual stress, can explain, among other phenomena, the appearance of dislocation pile-ups. The proposed evolution law consists of assuming nothing more that a linear relation between the inhomogeneity velocity gradient and the instantaneous value of the torsion of the (unique) material connection. That such a simple law can account for nonlinear phenomena is an encouraging sign of the power of the theory of continuous distributions of inhomogeneities, which is just beginning to be fully tapped. A possible extension of the theory would include the modelling of the release of residual stresses present in an isotropic solid. In this case, the dislocation density can be completely characterized by the curvature tensor of an appropriately defined Riemannian connection. The theory would be necessarily more involved than the one presented in this paper not only because the curvature tensor is of higher order than a torsion, but also because the evolution would involve a coupling with the solution of the equilibrium boundary-value problem at each instant. It is mainly for reasons of simplicity that we have limited the presentation to the solid crystal case.

2. Uniformity

Let $\mathfrak{B}$ denote an open, possibly unbounded, region in $\mathbb{R}^3$. We shall view it as a deformable continuum in a *reference configuration*. A *deformation* of the body $\mathfrak{B}$ is an embedding $\chi : \mathfrak{B} \to \mathbb{R}^3$. Its tangent map evaluated at the material point $X \in \mathfrak{B}$ is called the *deformation gradient* at X, and it will be denoted by $\mathbf{F}(X)$. In fact, due to the canonical identification of a tangent space of $\mathbb{R}^3$ with the Euclidean vector space E_3 we recognize the deformation gradient as an automorphism of E_3, and drop the explicit dependence of $\mathbf{F}$ on the material point X.

In pure elasticity the density of the stored energy per unit reference volume is given by a function $W(\mathbf{F}; X)$ where, as mentioned earlier, $\mathbf{F}$ is the gradient of the deformation from the reference configuration to the current configuration evaluated at X. Adopting a three dimensional vector space $\mathbf{V}$ as a *reference crystal* (an archetype material point) we say that the body $\mathfrak{B}$ is *materially uniform* whenever there exist smoothly distributed (throughout the body) *uniformity maps* $\mathbf{P}(X)$ from the reference crystal $\mathbf{V}$ to the tangent space of the reference configuration at X, and a real-valued function $\widehat{W}$ such that

$$W(\mathbf{F};X) = \widehat{W}(\mathbf{F}\mathbf{P}(X)) \tag{1}$$

for all deformation gradients $\mathbf{F}$ and any material point X, (Truesdell and Noll, 1965); see also (Elżanowski, Epstein and Śniatycki, 1990). Given a basis $\mathbf{E}_\alpha$ ($\alpha = 1,2,3$) in the reference crystal $\mathbf{V}$ and a (right-handed) coordinate system $\mathbf{e}_I$ ($I = 1,2,3$) in $\mathbb{R}^3$ the mappings $\mathbf{P}(X)$ induce in the reference configuration a field of bases

$$\mathbf{f}_\beta(X) \equiv P^I_\beta(X)\mathbf{e}_I. \tag{2}$$

called a *uniform reference*. The uniform frame at X is related to the uniform frame at Y by the linear isomorphism

$$\mathbf{P}(X;Y) \equiv \mathbf{P}(X)\mathbf{P}^{-1}(Y) \tag{3}$$

called a *material isomorphism* from Y to X. Note that the choice of the basis $\mathbf{E}_\alpha$ in the reference crystal, although arbitrary, has no effect on the choice of maps $\mathbf{P}(X;Y)$.

A uniform reference (a moving frame) $\mathbf{f}_\beta$ is not, in general, induced by any coordinate system on the body $\mathfrak{B}$ even if considered only in some neighborhood of a material point. However, if for every material point X there exists such a coordinate neighborhood (albeit different at different points) the body is called *locally homogeneous*, (Wang, 1967), (Wang and Truesdell, 1973). By an appropriate change of reverence configuration, the uniformity maps $\mathbf{P}(X)$ can then be chosen as independent of X in each such neighborhood. This in turn implies that the parallelism induced on $\mathfrak{B}$ by such a material reference $\mathbf{f}_\beta$ is locally trivial. The material connection associated with such a parallelism is torsion-free, where a *material connection* of the mathematical theory of inhomogeneities is a connection generated by any (homogeneous or not) uniform reference, (Noll, 1967). Note that any material connection is locally integrable, i.e., its curvature tensor vanishes locally, as uniform references are induced from the reference crystal by the smoothly distributed (throughout the body) mappings $\mathbf{P}(X)$.

For a *solid crystal* point the *material symmetry group* is finite. In particular, the *triclinic crystal* is a solid crystal with the trivial symmetry group (there are no symmetries other than the identity, say $\mathbf{I}$)[1]. A material body made of solid crystals has a unique material connection. This is in contrast with the case when the material symmetry group is continuous, e.g., in an isotropic solid.

[1] One may also allow $-\mathbf{I}$ to be a symmetry of a triclinic solid (Truesdell and Noll, 1965).

In this paper we shall only consider uniform material bodies made of triclinic crystals and such that there exists a global reference configuration in which all material isomorphisms $\mathbf{P}(X;Y)$ are proper rotations, i.e., the uniform reference corresponds to *c*ontorted aelotropy, (Noll, 1967) or, equivalently, a *s*tate of constant strain, (Epstein, 1987). This can be realized if, for example, there exists a global stress-free reference, and the reference crystal is assumed stress-free. Other states of stress are also possible. Indeed, one can show that in a 2-dimensional solid crystal body the state of stress compatible with a state of constant strain is hydrostatic, (Epstein, 1987).

In other words, if the body is in a state of constant strain, and if a (right-handed) orthonormal basis $\mathbf{e}_I$ $(I = 1, 2, 3)$ defines a Cartesian coordinate system on $\mathbb{R}^3$ then

$$\mathbf{f}_\beta(Z) = Q^I_\beta(Z)\mathbf{e}_I, \tag{4}$$

where all $Q^I_\beta(Z)$ are proper orthogonal tensors. The Christoffel symbols of the second kind of the unique (constant strain) material connection are given in the Cartesian coordinate system by

$$\Gamma^I{}_{KJ}(Z) = -Q^I_{\alpha,J}(Z)Q^\alpha_K(Z) \tag{5}$$

where "comma" indicates partial differentiation. When the body is locally homogeneous, and the rotations $Q^I_\beta(Z)$ are locally material point independent, the Christoffel symbols of the material connection vanish.

3. Evolution Law

Consider a uniform solid crystal body. In the realm of pure elasticity the given uniform reference remains unchanged. In other words, there are no processes of elastic deformations which may change the existing structure. However, anelastic processes involve usually mechanisms which modify the distribution of material inhomogeneities. This can be modelled by allowing the uniform reference to change in time. As the uniform reference $\mathbf{f}_\alpha$ evolves, and assuming that the evolution does not alter the symmetry group, its time derivative yields

$$\dot{\mathbf{f}}_\beta = \dot{P}^I_\beta \mathbf{e}_I = \dot{P}^I_\beta (P^{-1})^\gamma_I \mathbf{f}_\gamma = L^\gamma{}_\beta \mathbf{f}_\gamma, \tag{6}$$

as implied by relation (2). Here, $L^\gamma{}_\beta$ represent the components of the *inhomogeneity velocity gradient* (Epstein and Maugin, 1996)

$$\mathbf{L} \equiv \mathbf{P}^{-1}\dot{\mathbf{P}}, \tag{7}$$

which measures the temporal rate of change of uniform references pulled back to the reference crystal. Note that for the triclinic crystal body in a state of constant strain

$$L^{\gamma}_{\ \beta} = \dot{Q}^{I}_{\beta} Q^{\gamma}_{I} \tag{8}$$

are components of a skew-symmetric matrix, as implied by (4).

Given a particular uniform reference of an arbitrary uniform material body the *torsion*

$$T^{I}_{\ KJ} \equiv \Gamma^{I}_{\ KJ} - \Gamma^{I}_{\ JK} \tag{9}$$

of the induced material connection is an indicator of whether or not the body is homogeneous. Indeed, if the torsion vanishes the induced material parallelism is trivial and the body is homogeneous. On the other hand, if the torsion of a particular material connection does not vanish the corresponding uniform reference is not integrale. The body may still be homogeneous as there may exist another uniform reference, obtained by the action of the material symmetry group, inducing a flat material connection. In the triclinic crystal case, however, as we pointed out earlier, the material connection is unique. The torsion of such a material connection is not only an indicator of inhomogeneity but, it may be considered a true measure of the density of the distribution of inhomogeneities.

We, therefore, postulate that regardless of the state of stress the distribution (density) of inhomogeneities is the driving force behind the intrinsic anelastic evolution of these inhomogeneities. According to this idea we suggest an evolution law of the form:

$$\dot{\mathbf{P}}(X,t) = f(\mathbf{T}(X,t), \mathbf{P}(X,t)) \tag{10}$$

where $\mathbf{T}$ is the torsion tensor of the instantaneous intrinsic material connection (as generated by the current uniformity maps $\mathbf{P}$), and where f is assumed not to depend explicitly on $\mathbf{X}$ because of the assumed uniformity of the evolving body.[2] Note that (10), although particularly appealing in the triclinic crystal case, may as well be applicable in other situations with possible extra equivariance conditions.

Formulating an evolution law is a difficult constitutive modelling process. However, for such a law to describe a true evolution it must satisfy the *principle of covariance* (Epstein and Maugin, 1996). That is, it must be independent of any particular reference configuration chosen. If $\lambda : \mathbb{R}^3 \to \mathbb{R}^3$ is a diffeomorphism representing a change of

[2] Realize that the function f may be made to depend also on some other parameters like temperature, stress, etc.

reference configuration and $\mathbf{H}$ denotes its gradient at a material point the corresponding uniformity maps $\mathbf{R}$ and $\mathbf{P}$ are related by

$$\mathbf{R} = \mathbf{HP}. \tag{11}$$

As we want our evolution law to describe a particular physical situation in a manner independent from a reference configuration and, since λ is time independent

$$\dot{\mathbf{R}} = \mathbf{H}\dot{\mathbf{P}}. \tag{12}$$

This implies that

$$f(\mathbf{HTH}^{-1}\mathbf{H}^{-1}, \mathbf{HP}) = \mathbf{H}f(\mathbf{T}, \mathbf{P}) \tag{13}$$

for all non-singular tensors $\mathbf{H}$. Note that as the torsion $\mathbf{T}$ is a vector-valued two-form the notation $\mathbf{HTH}^{-1}\mathbf{H}^{-1}$ is a shorthand for the pull-back transformation whose coordinate representation takes the form

$$\hat{T}^I_{JK} = (H^{-1})^I_A T^A_{BC} H^B_J H^C_K. \tag{14}$$

In particular, let us select (with some abuse of notation) $\mathbf{H} = \mathbf{P}^{-1}$ and define

$$f_{\mathbf{v}}(\mathbf{T}) \equiv f(\mathbf{P}^{-1}\mathbf{TPP}, \mathbf{I}). \tag{15}$$

Hence,

$$\dot{\mathbf{P}} = \mathbf{P}f_{\mathbf{v}}(\mathbf{T}) = \mathbf{P}f(\mathbf{T}_{\mathbf{v}}, \mathbf{I}), \tag{16}$$

where

$$\mathbf{T}_{\mathbf{v}} \equiv \mathbf{P}^{-1}\mathbf{TPP} \tag{17}$$

can be recognized as a density of the distribution of inhomogeneities (torsion tensor) seen from the perspective of the reference crystal. The evolution equation (16) can now be rewritten in terms of the inhomogeneity velocity gradient as follows:

$$\mathbf{L}(\mathbf{P}) = f_{\mathbf{v}}(\mathbf{T}). \tag{18}$$

It is not difficult to see that this form of the evolution law is completely invariant.

In particular, we may restrict the form of the evolution law by supposing a linear relation such that

$$\mathbf{L}(\mathbf{P}) = \mathbf{CT}_{\mathbf{v}}, \tag{19}$$

where $\mathbf{C}$ is a fifth order tensor of material constants. In other words the evolution law is given in component form by

$$(P^{-1})^\alpha_I \dot{P}^I_\beta = C^{\alpha\ \ \sigma\lambda}_{\ \beta\rho} (P^{-1})^\rho_M P^N_\sigma P^K_\lambda T^M_{NK}. \tag{20}$$

According to the *principle of actual evolution* (Epstein and Maugin, 1996) a process described by such an evolution law is truly evolutive only if the inhomogeneity velocity gradient $\mathbf{L}$ is outside of the Lie algebra of the material symmetry group of the reference crystal. In the case of a material body made of triclinic crystals, when the material symmetry group is finite, this principle implies that every non-trivial evolution, i.e., $L^{\gamma}_{\ \beta} \neq 0$, represents a true evolution.

4. The two-dimensional case

For the sake of specificity and to illustrate the range of phenomena within the scope of this approach, we consider now a class of problems for which the uniform reference is independent at all times of, say, the third Cartesian coordinate. In doing so, we render the evolution problem two dimensional and gain the added computational simplicity afforded by the explicit representation of the rotation by means of a single angular parameter.

Adopting an orthonormal basis in $\mathbf{V}$ and a Cartesian coordinate system x, y, z in the fixed reference configuration, the assumption that at all times t and at all points the uniform reference represents a state of constant strain results in the following matrix representation of the uniformity maps $\mathbf{P}$:

$$[\mathbf{P}] = \begin{pmatrix} \cos\theta(x,y,t) & \sin\theta(x,y,t) & 0 \\ -\sin\theta(x,y,t) & \cos\theta(x,y,t) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{21}$$

where $\theta = \theta(x, y, t)$ measures, say, the counterclockwise rotation between the x-axis and the vector $\mathbf{f}_1$. The non-vanishing Christoffel symbols of of the second kind of the induced material connection $\Gamma^{I}_{\ KJ}$ can now be calculated directly from (5) as

$$\Gamma^{1}_{\ 21} = -\Gamma^{2}_{\ 11} = \theta_{,x} \tag{22}$$

$$\Gamma^{1}_{\ 22} = -\Gamma^{2}_{\ 12} = \theta_{,y} \tag{23}$$

whence the non-vanishing torsion components are:

$$T^{1}_{\ 12} = -T^{1}_{\ 21} = -\theta_{,x} \tag{24}$$

$$T^{2}_{\ 12} = -T^{2}_{\ 21} = -\theta_{,y}\,. \tag{25}$$

Similarly, the non-vanishing components of the inhomogeneity velocity gradient at the reference crystal are

$$L^1{}_2 = -L^2{}_1 = \theta_{,t}\,. \tag{26}$$

The most general evolution law (20) results (after some calculation effort) in the single quasi-linear partial differential equation

$$\theta_{,t} + (a\cos\theta - b\sin\theta)\theta_{,x} + (a\sin\theta + b\cos\theta)\theta_{,y} = 0, \tag{27}$$

where a and b are, respectively, the material constants $2C^1{}_{21}{}^{12}$ and $2C^1{}_{22}{}^{12}$. These are the only two material constants left due to the skew-symmetry of the torsion tensor and the form of the uniformity maps (21).

We may further simplify the form of the evolution equation (27) by writing it as a single nonlinear balance law for the new variable β

$$\beta_{,t} + c(\sin\beta)_{,x} - c(\cos\beta)_{,y} = 0, \tag{28}$$

where $\beta \equiv \theta + \theta_0$, $c = \frac{1}{\sqrt{a^2+b^2}}$, and where θ_0 is such that $\tan\theta_0 = \frac{b}{a}$.

The characteristic strips (Duff, 1956) of this equation are solutions of the following system of ordinary differential equations:

$$\frac{dt}{ds} = 1, \tag{29}$$

$$\frac{dx}{ds} = c\cos\beta, \tag{30}$$

$$\frac{dy}{ds} = -c\sin\beta, \tag{31}$$

$$\frac{d\beta}{ds} = 0, \tag{32}$$

$$\frac{d\beta_{,t}}{ds} = -c\beta_{,t}\left[\beta_{,x}\sin\beta + \beta_{,y}\cos\beta\right], \tag{33}$$

$$\frac{d\beta_{,x}}{ds} = -c\beta_{,x}\left[\beta_{,x}\sin\beta + \beta_{,y}\cos\beta\right], \tag{34}$$

$$\frac{d\beta_{,y}}{ds} = -c\beta_{,y}\left[\beta_{,x}\sin\beta + \beta_{,y}\cos\beta\right], \tag{35}$$

As it is well known, the quasi-linearity of the single partial differential equation has several important consequences. Firstly, for given initial conditions $x(0)$, $y(0)$, $t(0)$ and $\beta(x(0), y(0), 0)$, the first four equations can be solved independently from the last three. A line $x(s), y(s), t(s)$ thus obtained is called a *characteristic curve* or simply a *characteristic*. Equation (32) implies that β is constant along each characteristic. Moreover, the parameter s, according to (29), can be identified with time t, except for an arbitrary additive constant. Finally,

the constancy of β implies that along a characteristic the right-hand sides of equations (30) and (31) are constant, and therefore that the characteristics are actually straight lines. The values of the material constants, together with the initial condition, determine whether or not the characteristics will tend to converge (intersect) or diverge. In the former case, we will observe the creation of dislocation pile-ups, while the latter is a representation of the tendency of the dislocations to dissipate after the passage of a long enough time. Indeed, the general Cauchy problem for such a balance law has, as it is well known (Dafermos, 2000), no smooth global solution even for smooth compactly supported initial condition. A solution stays temporarily smooth but eventually develops singularities. The blow-up of a smooth solution, which in the context of our model we identify with a dislocation pile-up, occurs when the spatial gradient of β becomes unbounded. In a one-dimensional case, given any particular initial distribution of inhomogeneities, it is rather elementary to determine, as shown in (Elżanowski and Epstein, 2002), such propagation characteristics as the blow-up time, the speed of propagation (Rankine-Hugoniot condition), and the propagation condition for the amplitude of the pile-up. Moreover, looking at the Rankine-Hugoniot condition for the evolution equation (28), whether planar or one-dimensional, it is easy to realize a possibility of the occurrence of a stationary pile-up, i.e., a singular pattern of inhomogeneities which will not propagate.

5. Examples

For the sake of being even more specific and to be able to illustrate better any of the above mentioned types of evolutions let us restrict further our analysis to the one-dimensional case by assuming that the uniform references depend only on one Cartesian coordinate, say y. This renders the evolution equation particularly simple, namely:

$$\beta_{,t} + c\beta_{,y} \sin \beta = 0. \tag{36}$$

The general Cauchy problem for such a balance law has, as it is well known, no smooth global solution even for smooth compactly supported initial condition. A solution stays temporarily smooth but eventually develops singularities. The blow-up of a smooth solution, which in the context of our model we identify with the dislocation pile-up, occurs when $\beta_{,y}$ becomes unbounded. It is easy to show by integrating along characteristics that this is possible provided

$$c\beta_0' \cos \beta_0(y) < 0 \tag{37}$$

at some $y \in \mathbb{R}$, where $\beta_0(y) \equiv \beta(y,0)$ and where $k(y) \equiv c\cos\beta_0(y)$ is obviously constant along the characteristics. The actual breaking of a continuous solution will be observed at the critical time

$$t_c \equiv \min_y \frac{-1}{c\beta_0'(y)\cos\beta_0(y)}. \tag{38}$$

Such a singularity, once developed, will propagate, as implied by the Rankine-Hugoniot condition, with the speed

$$v = c\frac{[\cos\beta]}{[\beta]} \tag{39}$$

along the shock-curve $y = \Gamma(s)$, where $\frac{d}{ds}\Gamma(s) = v(y(s),s)$. The evolution of the amplitude $[\beta]$ of such a shock is given by the propagation condition

$$[\tilde{\beta}] = c\left(\frac{[\cos\beta]}{[\beta]}[\beta_{,y}] + [\beta_{,y}\sin\beta]\right), \tag{40}$$

where $[f(\beta)] \equiv f(\beta^+) - f(\beta^-)$ denotes the jump of the quantity f across the shock-curve Γ, and where $[\tilde{\beta}]$ indicates differentiation along Γ. Using the method of singular surfaces the propagation of such a singularity can be further analyzed by developing the infinite system of iterated compatibility conditions and solving it numerically.

To show the relation between the form of the initial condition and the choice of the material constants a and b we briefly discuss here some one-dimensional evolution initial-value problems.

(i) Suppose that $a = b = 1$ and let $\beta_0(y) = \arctan y$. As $\beta_{0,y} > 0$ the condition (37) is never satisfied proving that no pile-up of dislocation will ever occur. A simple analysis of characteristics shows, in fact, that the solution $\theta(y)$ tends asymptotically to $-\frac{\pi}{4}$ at every $y \in \mathbb{R}$.

(ii) Let $\beta_0(y) = -\arctan y$ and let us keep the same material constants. This initial condition, in contrast to the previous one, will develop, as easily attested by (37), into a shock. In fact, investigating the arrangement of characteristics and calculating the critical blow-up time (38) one arrives at the conclusion that the two shocks travelling in opposite directions (one front-shock and one back-shock) will develop at the same time $t_c = \frac{\sqrt{2}}{2}$.

(iii) Suppose $a = b = 1$ and select a symmetric (about $y = 0$) initial condition, e.g., $\beta_0(y) = \frac{\pi}{2}\operatorname{sech} y$. An elementary analysis of characteristics shows that this solution will blow-up in finite time into a front shock. Changing the material constants to $a = -b = -1$ but keeping the initial condition unchanged will make very little difference. Indeed, rewriting the evolution equation for the new material constants

as $\beta_{,t} + \frac{\sqrt{2}}{2}\beta_{,y}\cos\beta = 0$ one can easily conclude that the new solution also blows up in finite time. However, a different part of the initial condition contributes now to the pile-up, slowing down its occurrence and propagation considerably.

(iv) As the last example we consider the spherically symmetric planar problem. In other words, we seek solutions to the evolution equation (28) such that it is invariant at all times $t \geq 0$ with respect to rotations about the origin. Rewriting equation (28) in the polar coordinates (ϱ, ψ) we obtain

$$\beta_{,t} + c\beta_{,\varrho}\sin(\beta - \psi) - \frac{c}{\varrho}\beta_{,\psi}\cos(\beta - \psi) = 0, \tag{41}$$

where $\beta = \beta(\varrho, \psi, t)$. The solution β is truly rotationally invariant provided

$$(\beta - \psi)_{,\psi} = 0. \tag{42}$$

Hence,

$$\beta(\varrho, \psi, t) = \psi + F(\varrho, t), \tag{43}$$

where

$$F_{,t} + cF_{,\varrho}\sin F - \frac{c}{\varrho}\cos F = 0. \tag{44}$$

What we have now is a one-dimensional balance law with the source. The characteristic curves are no longer straight lines and the solution F is no longer constant along characteristics. The initial value problem is well posed only locally in time. As in the case of a conservation law the solution of (44) generally stays smooth only up to some critical time at which a singularity develops. Moreover, the source term may even cause the singular solution to become unbounded in finite time and, if dissipative enough, it may prevent all together the breaking of some relatively weak waves. Note also that for the source term of (44) plays a prominent role close to the origin while it is negligible very far away from the center. Indeed, the proximity of defects increases the density of defects which, in turn, as expected, influences their evolution in a more significant way.

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