

Exact solution for dislocation bowing and a posteriori numerical technique for dislocation touching-splitting

Petr Pauš^{1,2} and Shigetoshi Yazaki¹

¹ Meiji University, 1-1-1 Higashi-Mita, Tama-ku, Kawasaki, Kanagawa 214-8571, Japan

² Czech Technical University in Prague, Břehová 7, 115 19 Praha, Czech Republic

E-mail pausp@geraldine.fjfi.cvut.cz

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Abstract

In dislocation dynamics, dislocations can be regarded as open plane curves evolving according to the curvature flow with an external force. In the present paper, evolving curves connecting two circular obstacles are treated from both mathematical and numerical viewpoints: An exact solution curve is constructed with sliding endpoints along obstacles, and all important and typical phenomena including touching-splitting, non-touching and Orowan island can be treated numerically.

Keywords dislocation dynamics, touching-splitting phenomena, dislocation bowing, evolution curves, sliding endpoints along precipitates

Research Activity Group Mathematical Aspects of Continuum Mechanics

1. Introduction

Dislocation is a line defect of the crystalline lattice. Along the dislocation curve the regularity of the crystallographic arrangement of atoms is disturbed. The dislocation can be represented by a curve closed inside the crystal or by a curve ending on the crystal surface. The presence of dislocations and their interaction strongly influence many of material properties. Therefore, there is a strong interest in understanding and modeling their behavior without performing expensive experiments.

The mathematical model of the dislocation dynamics is based on the curvature flow equation with forcing term $\mathcal{B}V = \mathcal{F} - \mathcal{T}k$ for open or closed curves, where V is the normal velocity of the curve, k is the curvature, \mathcal{F} is the external forcing term, \mathcal{B} is the drag coefficient and \mathcal{T} is the line tension [1]. In a uniform or ideal crystal case, all parameters $\mathcal{B}, \mathcal{F}, \mathcal{T}$ can be taken as positive constants, then, under a suitable rescaling in time, the evolution equation can be rewritten as

$$V = C - k \quad (1)$$

for a positive constant C . According to this evolution law, the dislocation curves move toward circular obstacles (strong precipitates), then they touch the obstacles and bend in the direction, say \vec{v} , of a line perpendicular to the line connecting two obstacles [2]. See Fig. 1a. The curves seem to move along the obstacle. Hence, the evolving curve and the obstacle seem to have a common tangent line at the touching point. In the present paper, we call this observation *tangential criterion*. See Fig. 2. Between two obstacles, the similar bending phenomena may occur starting from the opposite two sides. As a result, one can observe the following two kinds of phenomena: two evolving curves touch each other (Fig. 1a, left-hand side), or converge to some curves without touching

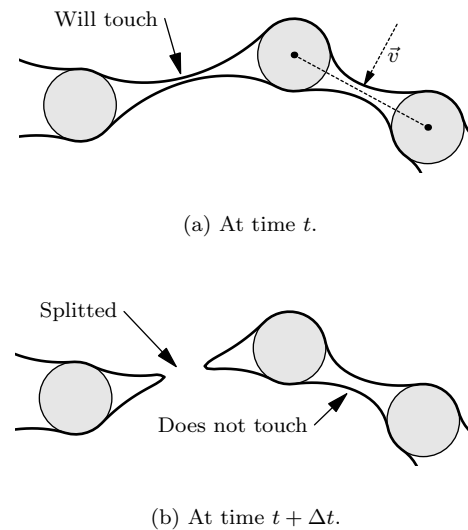


Fig. 1. Dislocation line along precipitates. The touching-splitting and non-touching phenomena are observed.

(Fig. 1a and 1b, right-hand side). In the former case, the two curves touch and split (Fig. 1b, left-hand side).

In the present paper, the touching-splitting and non-touching phenomena are treated from both mathematical and numerical points of view. In Section 2, to focus on these phenomena, a local coordinates will be introduced between two circular obstacles, that is, we will consider evolving open curves with two endpoints moving along each circle, and an exact solution will be constructed. To the best of our knowledge, no one has studied evolving curve connecting two circles; on the other hand, fixed-endpoints case has been studied extensively by various authors (e.g., [3–6]).

In Section 3, touching-splitting phenomena for planar

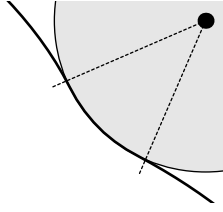


Fig. 2. Tangential criterion: dislocation line touching a precipitate.

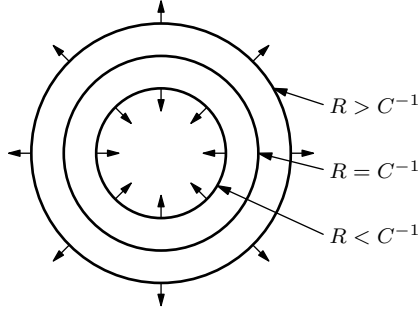


Fig. 3. Behavior of the circular solution.

curves will be treated from a numerical point of view. Under the so-called direct approach, we should estimate the touching time of two curves. Usually two curves are regarded touching each other, when the distance between them is less than a given tolerance. Such approach can be called a priori numerical technique [7] and there are essentially two difficult problems to solve: one, no one knows a reasonable value of tolerance, and two, one can not treat the case where two curves are very close each other, but they never touch. On the other hand, in our approach, when two curves touch or cross each other, splitting operation is performed. Therefore, our idea is simple and reliable, and the approach can be called *a posteriori numerical technique* in this sense.

2. Exact solution for dislocation bowing

In the case of closed solution curves, it is easy to obtain an exact circular solution with the radius R under the evolution equation $V = C - k$, since we have $V = dR/dt$ and $k = R^{-1}$. Solving $dR/dt = C - R^{-1}$, we obtain the exact solution

$$t = F(R(t)),$$

$$F(\rho) = \frac{1}{C} \left(\rho - R(0) + \frac{1}{C} \log \frac{C\rho - 1}{CR(0) - 1} \right), \quad (2)$$

which satisfies the following proposition (see Fig. 3).

Proposition 1 *We have the following properties:*

- if $R(0) > C^{-1}$, then $R(t) \rightarrow \infty$ holds as $t \rightarrow \infty$;
- if $R(0) < C^{-1}$, then there exists $T = F(0)$, such that $R(t) \rightarrow 0$ holds as $t \rightarrow T$.

By using an arc of the above circle solution, we will construct an exact solution of evolving open curve with moving endpoints on given circles.

Let $y = f(x, t)$ be a solution open curve. To construct an exact solution we assume that the solution curve is an arc of a circle with the radius $R(t)$ and the center

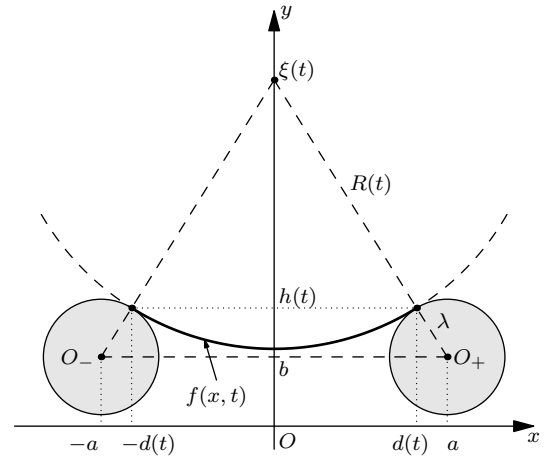


Fig. 4. Geometry settings.

$(0, \xi(t))$ as follows:

$$f(x, t) = \xi(t) - \sqrt{R(t)^2 - x^2} \quad (-d(t) < x < d(t)),$$

where the endpoints are $(\pm d(t), h(t))$ moving along two prescribed circular obstacles, say O_{\pm} , with the radius λ and the center (a, b) . Under the tangential criterion in Section 1, the exact circular solution can be constructed if $R(t)$ is a solution of

$$\frac{dR}{dt} = C - R^{-1}, \quad (3)$$

and

$$\xi(t) = b + \sqrt{(R(t) + \lambda)^2 - a^2},$$

$$d(t) = \frac{aR(t)}{R(t) + \lambda},$$

$$h(t) = f(\pm d(t), t),$$

where parameters and functions should satisfy

$$0 < a - \lambda < d(t) < a,$$

and $b \in \mathbb{R}$. See Fig. 4.

The minimum point, say $m(t)$, is achieved at $x = 0$, that is,

$$m(t) = f(0, t) = \xi(t) - R(t).$$

By virtue of Proposition 1, the following proposition holds.

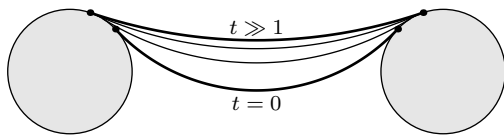
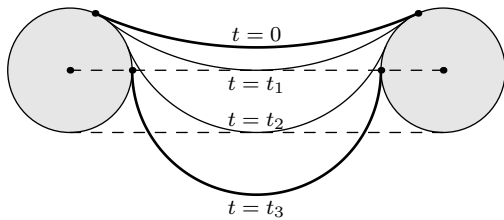
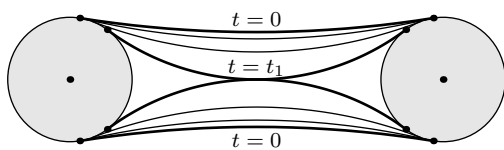
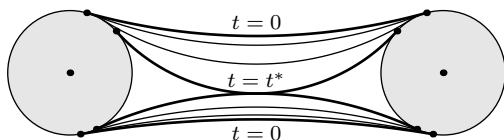
Proposition 2 *We have the following properties:*

- if $R(0) > C^{-1}$, then $m(t) \rightarrow b + \lambda$ holds as $t \rightarrow \infty$;
- if $R(0) < C^{-1}$ and $m(0) > b$, then there exist three breakpoints of time $0 < t_1 < t_2 < t_3 < T$ such that
 - ★ $m(t) \rightarrow b$ holds as $t \rightarrow t_1 = F(R_1)$,
 - ★ $m(t) \rightarrow b - \lambda$ holds as $t \rightarrow t_2 = F(R_2)$,
 - ★ $m(t) \rightarrow b + \lambda - a$ holds as $t \rightarrow t_3 = F(R_3)$,
 where

$$R_1 = \frac{a^2 - \lambda^2}{2\lambda}, \quad R_2 = \frac{a^2}{4\lambda}, \quad R_3 = a - \lambda,$$

and $T = F(0)$.

For example, if we choose $a = 1.5$, $b = 0.6$, $\lambda = 0.5$, $C = 0.75$, and $R(0) = 1.4$, we obtain the result corresponding to Fig. 5. Fig. 6 illustrates the result for


 Fig. 5. Exact solution, $R(0) > C^{-1}$.

 Fig. 6. Exact solution, $R(0) < C^{-1}$ and $m(0) > b$.

 Fig. 7. Symmetric solution, t_1 is the touching time.

 Fig. 8. Non-symmetric solution, t^* is the touching time.

the same geometry is chosen but this time $C = 0.05$ and $R(0) = 10$. According to Proposition 2, we obtain $R_1 = 2$, $R_2 = 1.125$, and $R_3 = 1$ computed from (2).

Symmetric or non-symmetric touching phenomena can be constructed by means of two exact solutions starting from opposite sides of obstacles. Fig. 7 illustrates the symmetric solution with the touching at $t_1 = F(R_1)$ according to Proposition 2. The non-symmetric solution is obtained by choosing different $R(0)$ for upper and bottom curve. See Fig. 8. We confirmed the exact solutions by numerical computation of (3).

3. Numerical treatment

We consider a simple, embedded and open plane curve Γ which is described by a smooth function $\vec{x} : [0, 1] \ni u \mapsto \vec{x}(u) \in \mathbb{R}^2$ with $|\partial_u \vec{x}(u)| > 0$, where $\vec{x}(0) \neq \vec{x}(1)$ are the two endpoints. We assume the total length of the curve Γ is finite. Here and hereafter, we denote $\partial_\xi F = \partial F / \partial \xi$ and $|\vec{a}| = \sqrt{\vec{a} \cdot \vec{a}}$ where $\vec{a} \cdot \vec{b}$ is the Euclidean inner product between vectors \vec{a} and \vec{b} in the plane \mathbb{R}^2 . The unit tangent vector can be defined as $\vec{t} = \partial_u \vec{x} / |\partial_u \vec{x}(u)| = \partial_s \vec{x}$, where s is the arc-length parameter and $ds = |\partial_u \vec{x}(u)| du$. The normal vector \vec{n} is defined in such a way that $\det(\vec{n}, \vec{t}) = 1$. The curvature k is defined by Frenet-Serret formula $\partial_s \vec{t} = -k \vec{n}$.

For a given simple, embedded, open plane curve $\Gamma_0 : \vec{x}_0(u)$ ($u \in [0, 1]$) with a finite length, our problem is to find a family of plane curves $\{\Gamma(t)\}_{0 \leq t < T}$, $T > 0$, where $\Gamma(t)$ is described by a smooth function

$$\vec{x} : [0, 1] \times [0, T] \ni (u, t) \mapsto \vec{x}(u, t) \in \mathbb{R}^2$$

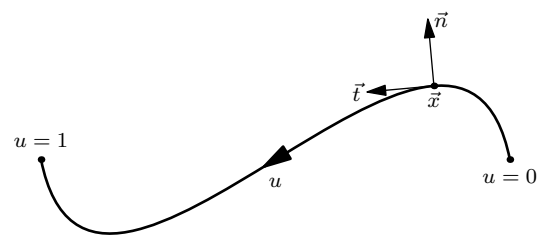


Fig. 9. Curve quantities.

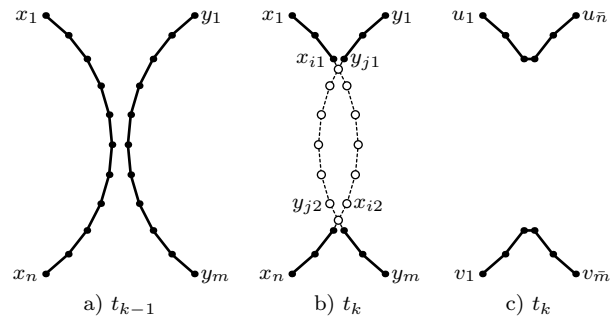


Fig. 10. Algorithm for topological changes.

with $|\partial_u \vec{x}(u, t)| > 0$, starting from $\Gamma(0) = \Gamma_0 : \vec{x}(u, 0) = \vec{x}_0(u)$ ($u \in [0, 1]$). It evolves in the normal and the tangential directions according to the following law:

$$\partial_t \vec{x} = V \vec{n} + \alpha \vec{t}. \quad (4)$$

Here $\vec{n} = \vec{n}(u, t)$ and $\vec{t} = \vec{t}(u, t)$ are the unit normal and tangential vectors, $V = C - k(u, t)$ and $\alpha = \alpha(u, t)$ are the normal and the tangential velocities, respectively, and $k(u, t)$ is the curvature. Note that the tangential velocity $\alpha(u, t)$, $u \in (0, 1)$ can be chosen arbitrary if α is continuous up to the endpoints [8].

Let us consider two open curves Γ_1 and Γ_2 discretized as $X = \{x_1, x_2, \dots, x_n\}$ and $Y = \{y_1, y_2, \dots, y_m\}$ in \mathbb{R}^2 . The curves evolve independently according to the equation (4). The algorithm for connecting two open curves is as follows:

1. At time t_k , find first two intersections of polygonal curves X and Y . If no intersection occurs, go to step 9.
2. Denote the starting points of intersecting line segments from X as x_{i1} , x_{i2} and from Y as y_{j1} , y_{j2} according to Fig. 10b.
3. Create two new open curves $U = \{u_1, u_2, \dots, u_{\bar{n}}\}$ and $V = \{v_1, v_2, \dots, v_{\bar{m}}\}$, where $\bar{n} = n - i2 + i1$ and $\bar{m} = m - j2 + j1$.
4. Copy points from X from x_1 up to x_{i1} to U .
5. Copy points from Y from y_{j1} up to y_1 to U .
6. Copy points from X from x_n up to x_{i2+1} to V .
7. Copy points from Y from y_{j2+1} up to y_m to V .
8. Delete X , Y and set $X = U$, $Y = V$. See Fig. 10c.
9. Proceed to a new time for X , Y , set $k = k + 1$, and go to step 1.

The main difference between this approach (checking the intersection of two curves) and standard known approach [7] (tolerance based connecting) is in its reliabil-

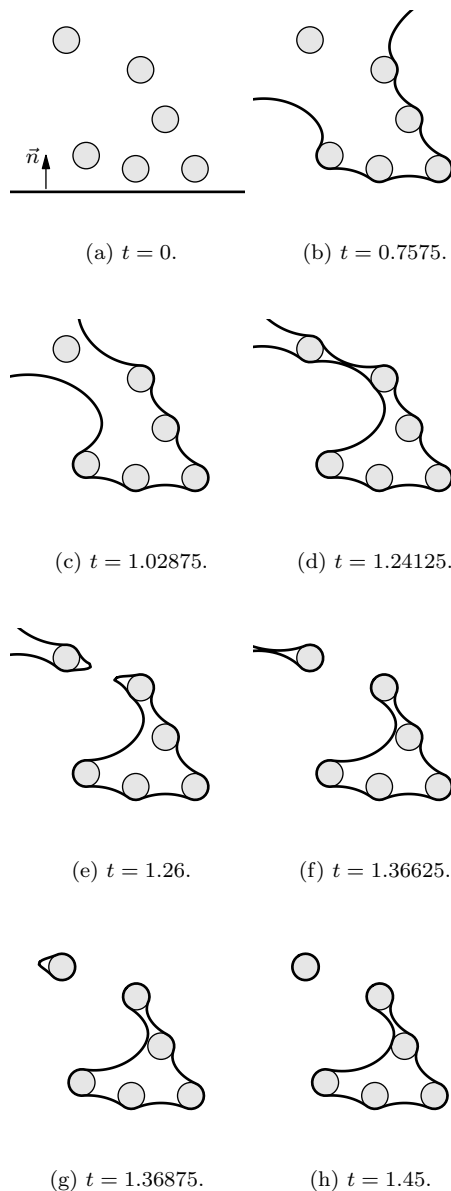


Fig. 11. Numerical solution of (4). Typical phenomena of topological changes and a bottleneck can be observed, namely the touching-splitting, non-touching, and the Orowan island.

ity. There is not any tolerance and also any artificial condition on the time step length. Curves can be discretized by less points and still the algorithm works well.

Fig. 11 indicates the numerical solution of (4) with a non-trivial tangential velocity α for numerical stability [8, 9]. The fixed endpoints and some parts of the curve are cropped from the figure to focus on the interaction with precipitates. All important and typical phenomena can be observed, namely the touching-splitting, non-touching, and the Orowan island [10].

4. Concluding remarks

In the present paper, evolving curves connecting two circular obstacles were treated by the evolution law $V = C - k$. An exact solution curve was constructed and a posteriori numerical technique was proposed. Under our numerical technique, one can treat touching-splitting

phenomena of two curves without a priori artificial criterion.

Future work remains as follows: (1) to treat general solution curves (other than circular arcs) for dislocation bowing from mathematical point of view, (2) to optimize the algorithm for topological changes, and (3) to establish the maximum principle for evolving open curves with prescribed moving endpoints.

Acknowledgments

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