Dislocation-density kinematics: a simple evolution equation for dislocation density involving movement and tilting of dislocations[§]

A.H.W. Ngan

Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong, P.R. China

Abstract

In this letter, a simple evolution equation for dislocation densities moving on a slip plane is proven. This equation gives the time evolution of dislocation density at a general field point on the slip plane, due to the approach of new dislocations and tilting of dislocations already at the field point. This equation is fully consistent with Acharya's evolution equation and Hochrainer et al.'s "continuous dislocation dynamics" (CDD) theory. However, it is shown that the variable of dislocation curvature in CDD is unnecessary if one considers one-dimensional flux divergence along the dislocation velocity direction.

[§] Research Letter invited by Editor of MRS Communications, based on invited presentation at 2017 MRS Spring Meeting.

Introduction

In the past two decades, tremendous progress has been made on developing theories for the kinematics of dislocation densities [1-4]. Of special importance is the equation $\dot{\boldsymbol{\alpha}} = -\vec{\nabla} \times (\boldsymbol{\alpha} \times \vec{v})$ for the evolution of the Nye tensor [5] $\boldsymbol{\alpha}$ proposed initially by Kröner [6] and further developed by Acharya [1], and a "continuous dislocation dynamics" (CDD) theory proposed by Hochrainer and co-workers [4], in which the key concept is the involvement of dislocation curvature as a second field variable in addition to dislocation density itself. However, there has been no documented attempt to reconcile these two important theories. Recently, the present author has also proposed an evolution scheme for dislocation densities based on consideration of the approach and tilting of single dislocations forming the dislocation densities [7]. In this paper, we show that Leung and Ngan's scheme [7] is fully consistent with Acharya's equation [1] and the CDD theory [4]. Moreover, we show that the curvature variable in CDD is unnecessary if divergence of dislocation flux is counted one dimensionally along the dislocation velocity direction, rather than two-dimensionally over the slip plane as in the CDD. Furthermore, we also present a clear delineation of how discrete dislocations would form coarse-grained densities, and how the evolution of densities can be derived from the movement of the comprising individual dislocations – this is an aspect which is not clear in Acharya's equation which deals only with geometrically necessary dislocations.

Before we begin, a note on nomenclature will be useful. First, by a "discrete" dislocation representation, we mean a single dislocation without any description of the evolution of the dislocation core itself. A "discrete" dislocation therefore has its contents represented by a delta-like function that does not change shape with space or time as the entire dislocation moves, and is therefore different from an "intensive" dislocation representation in which the Burgers vector distribution in the dislocation core is described in detail as in the Peierls-Nabarro model. In this paper, we will first derive the evolution of discrete dislocations in terms of their density fields, before we consider the evolution of coarse-grained dislocation densities.

Secondly, by "dislocation density", we refer to the number of dislocations threading unit area, which is a vector quantity with unit m^{-2} since the unit area is specified by its normal direction. This "area" definition is that used in the Nye tensor [1], which is the Burgers vector content threading unit area. Consider a group of dislocations which are momentarily straight and parallel to each other within a small pixel of the slip plane (FIG. 1). For an area A perpendicular to the dislocation lines, the area density of dislocations is therefore:

$$\rho = N/A \tag{1}$$

Since A is perpendicular to the dislocations, the ρ defined this way is not only the area density, but also the volume density of dislocation length per unit volume (a scalar). This can be seen by considering the dislocation length inside a control volume of $A \times d\xi$ where $d\xi$ is a small length along the dislocation direction $\hat{\xi}$. For areas A_1 and A_2 perpendicular to two orthonormal axes $\hat{x}_1$ and $\hat{x}_2$ generally placed on the slip plane, respectively, the same N dislocations correspond to area densities:

$$\rho_1 = \frac{N}{A/(\hat{\xi}\cdot\hat{x}_1)} = \rho\left(\hat{\xi}\cdot\hat{x}_1\right) = \vec{\rho}\cdot\hat{x}_1; \quad \rho_2 = \vec{\rho}\cdot\hat{x}_2 \tag{2a}$$

where the vector $\vec{\rho}$ is defined as $\vec{\rho} = \rho\, \hat{\xi}$. Since the factors $\hat{\xi} \cdot \hat{x}_1$ and $\hat{\xi} \cdot \hat{x}_2$ are ≤ 1, ρ_1 and ρ_2 are $\leq \rho$, and since $\hat{x}_1$ and $\hat{x}_2$ are arbitrary orthonormal directions on the slip plane, ρ as defined in eqn. (1) (with A being the area normal to the dislocations) is the maximum possible area density. Eqn. (2a) also implies that

$$\vec{\rho} = \rho_1 \hat{x}_1 + \rho_2 \hat{x}_2; \quad \rho = |\vec{\rho}| = \sqrt{\rho_1^2 + \rho_2^2} \tag{2b}$$

Eqn. (2a), which can be further written in the form

$$\rho_j = \rho\left(\hat{\xi} \cdot \hat{x}_j\right), \tag{2c}$$

gives the relation between a general area density ρ_j (number of dislocations threading unit area normal to $\hat{x}_j$) and the volume density ρ. When $\hat{x}_j$ is along $\hat{\xi}$, $\rho_j = \rho$ which is also the maximum area density.

In the following, we will first discuss Acharya's equation and modify it into a form more useful for our next development. Then, we will discuss the density vector field of discrete dislocations as proposed by Leung and Ngan [7], and prove that it satisfies Acharya's equation [1]. We will then derive the coarse-grained densities of dislocations and their evolution equation based on combined contributions from discrete dislocations. Then, finally, we will show that the evolution equation for coarse-grained densities is consistent with CDD [4].

Evolution equation for Nye's tensor

The kinematics of line objects moving in and out of threaded areas over which line densities are counted is encountered in classical physics such as electromagnetic induction. The well-known Maxwell-Faraday equation can be cast in the following form $\partial\vec{B}/\partial t = -\vec{\nabla} \times \left(\vec{B} \times \vec{v}\right)$ for the magnetic flux lines $\vec{B}$ movng with velocity $\vec{v}$. This equation applies equally well to dislocations [1, 6]; thus, in terms of the dislocation density and Nye tensor [5], their evolution equations are respectively:

$$\dot{\vec{\rho}} = -\vec{\nabla} \times (\vec{\rho} \times \vec{v}) \tag{3}$$

and

$$\dot{\boldsymbol{\alpha}} = -\vec{\nabla} \times (\boldsymbol{\alpha} \times \vec{v}) \tag{4}$$

where the Nye tensor is such that

$$\alpha_{ij} = b_i \rho_j, \quad \text{or} \quad \boldsymbol{\alpha} = \vec{b} \otimes \vec{\rho} \tag{5}$$

which gives the Burgers vector b_i along i threading unit plane with normal j. In eqn. (4), it is understood that the cross product in $\boldsymbol{\alpha} \times \vec{v}$ is between each row i of $\boldsymbol{\alpha}$ and $\vec{v}$, i.e. $(\boldsymbol{\alpha} \times \vec{v})_{il} = \alpha_{ij} v_k \epsilon_{ijl} \hat{x}_l$, or $\boldsymbol{\alpha} \times \vec{v} = \left(\vec{b} \otimes \vec{\rho}\right) \times \vec{v} = \vec{b} \otimes (\vec{\rho} \times \vec{v})$, and the curl "$\vec{\nabla}\times$" also operates on each row of the tensor $\boldsymbol{\alpha} \times \vec{v}$ – such operations on each row i of $\boldsymbol{\alpha}$ deal with the conservation of each component b_i of the Burgers vector contents carried by the dislocation lines as they move in space. With these, eqn. (4) is mathematically compatible with eqn. (3): in eqn. (4), $\dot{\boldsymbol{\alpha}} = \vec{b} \otimes \dot{\vec{\rho}}$ and $\boldsymbol{\alpha} \times \vec{v} = \left(\vec{b} \otimes \vec{\rho}\right) \times \vec{v} = \vec{b} \otimes (\vec{\rho} \times \vec{v})$, and hence, eqn. (4) becomes

$$\dot{\boldsymbol{\alpha}} = \vec{b} \otimes \dot{\vec{\rho}} = -\vec{\nabla} \times \left[\vec{b} \otimes (\vec{\rho} \times \vec{v})\right] = -\vec{b} \otimes \left[\vec{\nabla} \times (\vec{\rho} \times \vec{v})\right]$$

which then reduces to eqn. (3) by crossing out the constant $\vec{b}$ from both sides of the equation.

For dislocations gliding on a slip plane with normal $\hat{n}$, the dislocation velocity $\vec{v}$ has to be perpendicular to the dislocation line $\hat{\xi}$ and lying on the slip plane, i.e.

$$\vec{v} = v\left(\hat{n} \times \hat{\xi}\right) \tag{6}$$

where v is the magnitude of $\vec{v}$. Therefore, $\vec{\rho} \times \vec{v} = \rho v\, \hat{n}$, and so eqn. (3) reduces to

$$\dot{\vec{\rho}} = -\vec{\nabla} \times (\rho v\, \hat{n}) \tag{7}$$

Eqn. (7) is the evolution equation for the dislocation density on a single slip plane, based on the general conservation law in eqn. (3), as well as the condition of orthogonal movement of dislocations in eqn. (6). With the Cartesian coordinates shown in FIG. 1, $\hat{x}_3 = \hat{x}_1 \times \hat{x}_2$ is the slip plane normal $\hat{n}$, and hence eqn. (7) gives

$$\dot{\vec{\rho}} = \dot{\rho}_1 \hat{x}_1 + \dot{\rho}_2 \hat{x}_2 = -\frac{\partial(\rho v)}{\partial x_2}\hat{x}_1 + \frac{\partial(\rho v)}{\partial x_1}\hat{x}_2,$$

or,

$$\dot{\rho}_1 = -\frac{\partial(\rho v)}{\partial x_2}; \quad \dot{\rho}_2 = \frac{\partial(\rho v)}{\partial x_1}; \qquad \rho = \sqrt{\rho_1^2 + \rho_2^2} \tag{8}$$

Eqn. (8) automatically guarantees dislocation connectivity governed by $\vec{\nabla} \cdot \vec{\rho} = 0$. To see this, eqn. (8) readily gives

$$\vec{\nabla} \cdot \dot{\vec{\rho}} = -\frac{\partial^2(\rho v)}{\partial x_1 \partial x_2} + \frac{\partial^2(\rho v)}{\partial x_1 \partial x_2} = 0 \tag{9}$$

Hence, given that $\vec{\nabla} \cdot \vec{\rho} = 0$ at time $t = 0$, then $\vec{\nabla} \cdot \vec{\rho} = 0\ \forall t$. Furthermore, Eqn. (8) indicates that the flux ρv serves as the stream function for the density flow $\dot{\vec{\rho}}$. From eqn. (8), $\dot{\vec{\rho}} \cdot \vec{\nabla}(\rho v) = (\dot{\rho}_1 \hat{x}_1 + \dot{\rho}_2 \hat{x}_2) \cdot (\dot{\rho}_2 \hat{x}_1 - \dot{\rho}_1 \hat{x}_2) = 0$, which means that $\dot{\vec{\rho}}$ is perpendicular to $\vec{\nabla}(\rho v)$, or $\dot{\vec{\rho}}$ points along constant (ρv) curves.

While eqn. (4) provides a very general evolution law for the Nye tensor $\boldsymbol{\alpha}$, to clearly delineate the effects of GNDs versus those of the SSDs, Acharya and Roy [8] coarse-grained eqn. (4) into:

$$\langle \dot{\boldsymbol{\alpha}} \rangle = -\vec{\nabla} \times (\langle \boldsymbol{\alpha} \times \vec{v} \rangle) = -\vec{\nabla} \times (\langle \boldsymbol{\alpha} \rangle \times \langle \vec{v} \rangle + \boldsymbol{L^p}) \tag{10}$$

where $\langle \cdots \rangle = \langle \cdots \rangle(\vec{r}, t)$ denotes a coarse-grained average of quantity $(\cdots)$, namely, an average of $(\cdots)$ over a small space and time domain about the field point $\vec{r}$ and time t, and $\boldsymbol{L^p}$ is defined as $\langle \boldsymbol{\alpha} \times \vec{v} \rangle - \langle \boldsymbol{\alpha} \rangle \times \langle \vec{v} \rangle$. $\langle \boldsymbol{\alpha} \rangle$ therefore represents the GND contents of the dislocation population, and $\boldsymbol{L^p}$ represents the flux of the SSDs. However, the evolution of $\boldsymbol{L^p}$ is not exactly known, and so far, only phenomenological laws were used to describe it [8,9].

Density field for discrete dislocation on slip plane

While Acharya's eqn. (10) serves to by-pass detailed consideration of the kinematics of the individual dislocations comprising a dislocation density, it is thought here that defining clearly the relationship between the properties of the coarse-grained dislocation density and those of the comprising discrete dislocations is indeed very important for a density-based theory. It is therefore the purpose of this section to first derive the evolution of the density field of discrete dislocations, so that, in the next section, the evolution of dislocation densities can be derived.

Consider a general curved dislocation *i* lying on the slip plane as shown in FIG. 2(a,b). Leung and Ngan [7] recently proposed the following vector field of the dislocation density

$$\vec{\rho}_i(\vec{r}) = \delta(r_i')\hat{\xi}_i/b = \delta(r_i')(\sin\theta_i\,\hat{e} + \cos\theta_i\,\hat{s})/b \tag{11}$$

where $\vec{r} = (x, y)$ is a general field point on the slip plane, r_i' is the shortest (perpendicular) distance from $\vec{r}$ to the dislocation curve, $\hat{\xi}_i = (\sin\theta_i\,\hat{e} + \cos\theta_i\,\hat{s})$ is the local tangent direction of the dislocation at the point closest to $\vec{r}$ with θ_i being the dislocation character there, b is the atomic thickness of the slip plane, and $\delta(r_i')$ is a delta-like function that describes the core distribution of the dislocation. Essentially, eqn. (11) says that the vector field $\vec{\rho}_i(\vec{r})$ is zero everywhere except when on the dislocation line ($r_i' = 0$) where $\vec{\rho}_i = \hat{\xi}_i/b$. (The b here is to ensure that $|\vec{\rho}_i|$ has the meaning of one dislocation per cross section of the slip plane.)

Here, we show that eqn. (11) satisfies eqn. (7) or (8). By re-writing eqn. (11) as

$$\vec{\rho}_i(\vec{r}) = \rho_i(r_i')\hat{\xi}_i \tag{12}$$

where $\rho_i(r_i') = \delta(r')/b$, its time derivative is:

$$\dot{\vec{\rho}}_{\boldsymbol{i}} = \underbrace{-\,\rho_i'(r_i')v_i\,\hat{\xi}_i}_{\textit{approach}} + \underbrace{\rho_i(r_i')\,\dot{\hat{\xi}}_i}_{\textit{tilting}} \tag{13}$$

where $\rho_i'(r_i') = d\rho_i(r_i')/dt = \delta'(r_i')/b$, $-\partial r_i'/\partial t$ is written as v_i which has the meaning of the velocity the dislocation approaches the field point $\vec{r}$ (FIG. 2(a)). Without loss of generality, we choose the coordinate system to be $\hat{x}_2 = \hat{\xi}_i$, and $\hat{x}_1 = \left(\hat{\xi}_i \times \hat{n}\right)$ which points along the negative v_i direction (see FIG. 2(b)). Then, for the vector field defined in eqn. (11), eqn. (8) gives

$$\begin{aligned}\dot{\vec{\rho}}_{\boldsymbol{i}} &= -\frac{\partial(\rho_i v_i)}{\partial x_2}\hat{x}_1 + \frac{\partial(\rho_i v_i)}{\partial x_1}\hat{x}_2 \\ &\qquad = -\rho_i\,\frac{dv_i}{d\xi_i}\left(\hat{\xi}_i \times \hat{n}\right) - v_i\,\rho_i'(r_i')\frac{\partial r_i'}{\partial x_2}\left(\hat{\xi}_i \times \hat{n}\right) - \rho_i\frac{\partial v_i}{\partial x_1}\hat{\xi}_i - v_i\,\rho_i'(r_i')\,\hat{\xi}_i\end{aligned}$$

(14)

since $x_2 = \xi_i$ which is the coordinate along the dislocation line, and $x_1 = -r_i'$. It is important to note that the $\partial/\partial x_1$ and $\partial/\partial x_2$ operators in eqn. (14) involve displacing the field point $\vec{r}$ by either ∂x_1 or ∂x_2 along $\hat{x}_1$ or $\hat{x}_2$ respectively while the dislocation stays stationary. Hence, v_i being the velocity of the dislocation is independent of the position of the field point $\vec{r}$ along r_i', and so in eqn. (14), $\partial v_i/\partial x_1 = 0$. For the $\partial r_i'/\partial x_2$ term, we consider the general case of the dislocation exhibiting a local radius of curvature R. From geometry shown in FIG. 2(b), if the field point $\vec{r}$ moves by ∂x_2 along $\hat{x}_2$, the resultant change $\partial r_i'$ in the perpendicular distance to the dislocation r_i' is given by

$$R - (r_i' + \partial r_i') = \sqrt{(R - r_i')^2 + \partial x_2^2}, \quad \text{or} \quad \frac{\partial r_i'}{\partial x_2} = \frac{-\partial x_2}{\sqrt{(R-r_i')^2 + \partial x_2^2} + (R - r_i')}$$

Thus, unless $r_i' = R$, i.e. the field point $\vec{r}$ is at the center of curvature which would certainly be problematic, $\partial r_i'/\partial x_2 = 0$. Therefore, eqn. (14) becomes

$$\dot{\vec{\rho}}_{\boldsymbol{i}} = -\rho_i \, \frac{dv_i}{d\xi_i} \big(\hat{\xi}_i \times \hat{n}\big) - v_i \, \rho_i'(r_i') \, \hat{\xi}_i$$

Furthermore, from FIG. 2(a), $(dv_i/d\xi_i)\big(\hat{\xi}_i \times \hat{n}\big) = \dot{\theta}_i\big(\hat{\xi}_i \times \hat{n}\big) = -\,\dot{\hat{\xi}}_i$, and so the above equation becomes

$$\dot{\vec{\rho}}_{\boldsymbol{i}} = \rho_i \, \dot{\hat{\xi}}_i - v_i \, \rho_i' \, \hat{\xi}_i$$

which is eqn. (13). Hence, the $\vec{\rho}_i(\vec{r})$ defined in eqn. (11) or (12) satisfies eqn. (7) and is a valid representation of the density field of a general dislocation. Moreover, eqn. (13) gives the time evolution of the dislocation density field, and when cast in this form, the evolution does not contain the curvature as an explicit variable, as in the case of CDD [4]. The local curvature does affect the velocity v_i due to line tension effects, but this would be a dynamics consideration rather than a kinematics one.

We further analyze the two terms in eqn. (13). The second term in eqn. (13), $\rho_i(r_i') \, \dot{\hat{\xi}}_i$, is obviously the change due to tilting of the dislocation on the slip plane when it is already at the field point $\vec{r}$ (so that $\rho_i(r_i')$ is non-zero). The first term $-v_i \, \rho_i' \, \hat{\xi}_i$ is due to the approach of the dislocation towards the field point $\vec{r}$. To see this, consider FIG. 3. The definition of ρ_i, as quantity of dislocation threading unit plane perpendicular to dislocation line, is such that $b\rho_i \, dr_i'$ is the quantity of dislocation within a small distance dr_i' on the slip plane the thickness of which is b. During time δt, the quantity of dislocation that has passed through the point r' from the dislocation

$$= b \int_{r_i'}^{r_i' - v_i \, \delta t} \rho_i(r') \, dr' = b\rho_i(r_i') v_i \, \delta t \,,$$

and the quantity of dislocation that has passed through the point $r_i' + dr_i'$ from the dislocation

$$= b\rho_i(r_i' + dr_i') v_i \, \delta t$$

The increase in dislocation quantity between r_i' and $r_i' + dr_i'$ is therefore:

$$b\,\dot{\rho}_i\,\delta t\,dr_i' = b\,v_i\,\delta t\,[\rho_i(r_i') - \rho_i(r_i' + dr_i')]$$

or

$$\dot{\rho}_i = -v_i\,\rho_i'(r_i')$$

This increase in dislocation quantity at r_i' all bears the line direction $\hat{\xi}_i$, and so the corresponding change in the dislocation-density vector at r_i' is $\dot{\vec{\rho}}_i = -\rho_i'(r_i')v_i\,\hat{\xi}_i$, which is actually the first term in eqn. (13). It is also easy to see that, since $\dot{\hat{\xi}}_i \cdot \hat{\xi}_i = \dot{\theta}_i(\sin\theta_i\,\hat{s} - \cos\theta_i\,\hat{e}) \cdot (\sin\theta_i\,\hat{e} + \cos\theta_i\,\hat{s}) = 0$, the two terms in eqn. (13) are orthogonal to one another, with the approach and tilting term parallel and normal to $\hat{\xi}_i$ respectively.

Kinematics of coarse-grained dislocation distribution on a single slip plane

In FIG. 3, the $\rho_i(r_i')$ function for a discrete dislocation *i* does not change shape as the dislocation moves with velocity v_i. When attempting to generalize to a coarse-grained distribution of dislocations of the same slip system, the contents of the distribution may move with different speeds so that the overall profile may change shape; therefore, eqn. (13) is not applicable to the coarse-grained picture by simply replacing the $\rho_i(r_i')$ there by $\rho(r')$ for the coarse-grained distribution. For the coarse-grained case, we have to go back to the more general form in eqn. (7): $\dot{\vec{\rho}} = -\vec{\nabla} \times (\rho v\,\hat{n})$. However, using this equation, or the original forms in eqns. (3) or (4), to represent a coarse-grained distribution in a straight-forward way would have the SSD components lost. To preserve the SSD contents, the evolution of each character $\hat{\xi}_\theta = \sin\theta\,\hat{e} + \cos\theta\,\hat{s}$ of the dislocation distribution has to be known, and this is the purpose here.

Let $\varrho(\vec{r},\theta)$ be the density of dislocations with character $\hat{\xi}_\theta = \sin\theta\,\hat{e} + \cos\theta\,\hat{s}$ at point $\vec{r}$, $0 \le \theta \le 2\pi$ (FIG. 4). Specifically, $\varrho(\vec{r},\theta)d\theta$ gives the density of dislocations of character θ to $\theta + d\theta$ at point $\vec{r}$. Through $\varrho(\vec{r},\theta)$, each character component of the total dislocation distribution is known, so $\varrho(\vec{r},\theta)$ serves the important role of preserving the SSD contents. Without loss of generality, consider the contribution of only dislocations with character θ to the change in the dislocation-density vector $\vec{\rho}$ at a particular field point. Choosing the coordinate system to be $\hat{x}_2 = \hat{\xi}_\theta$, and $\hat{x}_1 = \hat{\xi}_\theta \times \hat{n}$, eqn. (10) gives this contribution as

$$\dot{\vec{\rho}}\Big|_\theta = -\frac{\partial(\varrho v)}{\partial x_2}\hat{x}_1 + \frac{\partial(\varrho v)}{\partial x_1}\hat{x}_2 = -\varrho\frac{dv}{d\xi_\theta}\left(\hat{\xi}_\theta \times \hat{n}\right) - v\frac{\partial\varrho}{\partial\xi_\theta}\left(\hat{\xi}_\theta \times \hat{n}\right) + \frac{\partial(\varrho v)}{\partial x_1}\hat{\xi}_\theta$$

where ξ_θ is the coordinate along $\hat{\xi}_\theta$. By the same consideration as in FIG. 2(b), $\partial\varrho/\partial\xi_\theta = 0$, and by defining $r_{\hat{\theta}} = -x_1$ which points along the $\vec{v}$ direction (and hence the opposite $\hat{x}_1$ direction $\hat{\theta} = \hat{n} \times \hat{\xi}_\theta$, or circumferential direction in the positive sense of θ, see eqn. (6)), and writing $dv/d\xi_\theta$ as v_θ which represents the speed of tilting of the dislocation density, the above equation reduces to

$$\dot{\vec{\rho}}\Big|_{\theta}(\vec{r}) = -\underbrace{\frac{\partial(\varrho v)}{\partial r_{\hat{\theta}}}\hat{\xi}_{\theta}}_{movement} - \underbrace{\varrho(\vec{r},\theta)\, v_{\theta}\left(\hat{\xi}_{\theta} \times \hat{n}\right)}_{tilting} \tag{15}$$

This equation gives the change in the dislocation density-vector $\vec{\rho}$ at $\vec{r}$, due to the movement of dislocations of character θ towards and away from $\vec{r}$ (the movement term), and the tilting of dislocations initially with character θ already situated at $\vec{r}$ (the tilting term). As explained above, the purpose here is not to sum the $\dot{\vec{\rho}}\big|_{\theta}$ in eqn. (15) over all θ, since if this is done, the resultant would only be a change in the GND at $\vec{r}$ with the SSD contents lost. Instead, we note that $\dot{\vec{\rho}}\big|_{\theta}(\vec{r})$ corresponds to the change in ϱ itself at θ. The movement term in eqn. (15) is easy to see – this term brings in, or take away, dislocation contents with line direction $\hat{\xi}_{\theta}$ to or from $\vec{r}$, and so this results in a change in ϱ at θ due to dislocation movements. Writing

$$\dot{\varrho} = \dot{\varrho}^{move} + \dot{\varrho}^{tilt}, \tag{16}$$

we have, from the first term in eqn. (15),

$$\dot{\varrho}^{move} = -\frac{\partial(\varrho v)}{\partial r_{\hat{\theta}}} \tag{17}$$

The tilting term $\dot{\varrho}^{tilt}$ in eqn. (16) arises from the second term in eqn. (15), but in a less obvious way. The tilting term in eqn. (15) says that the θ-content of dislocations at $\vec{r}$ will be lost at a rate $\varrho(\vec{r},\theta)\, v_{\theta}|_{\theta}$ due to dislocations of character θ rotating to a higher angle. However, applying eqn. (15) to the character $\theta - d\theta$ would give $\varrho(\vec{r},\theta - d\theta)\, v_{\theta}|_{\theta-d\theta}$ as a rate of gain of the θ-content of dislocations at $\vec{r}$, due to rotation of dislocations with an initially lower character now to θ. Hence, during time δt, the total change in the θ-content of dislocations at $\vec{r}$ due to rotation is $\delta\varrho^{tilt} d\theta = -\varrho(\vec{r},\theta)\, v_{\theta}|_{\theta}\delta t\; + \varrho(\vec{r},\theta - d\theta)\, v_{\theta}|_{\theta-d\theta}\delta t$, and so

$$\dot{\varrho}^{tilt} = -\frac{\partial(\varrho v_{\theta})}{\partial\theta} \tag{18}$$

The resultant evolution equation for $\varrho(\vec{r},\theta)$ is therefore

$$\dot{\varrho}(\vec{r},\theta) = -\underbrace{\frac{\partial(\varrho v)}{\partial r_{\hat{\theta}}}}_{movement} - \underbrace{\frac{\partial(\varrho v_{\theta})}{\partial\theta}}_{tilting} \tag{19}$$

Here, as explained before, for a given θ of the dislocation character space, $r_{\hat{\theta}}$ is the coordinate along $\hat{\theta} = \hat{n} \times \hat{\xi}_{\theta}$ which is the circumferential direction in the positive sense of θ on the slip plane.

Instead of using eqn. (7), there is an independent way of proving eqn. (19), involving a density-distribution function for single dislocations of a similar nature as eqn. (11). Rather than specifying the density field of a single dislocation as a vector field as in eqn. (11), we may also specify it in terms of a $\varrho(\vec{r},\theta)$ function which is now a scalar field for the dislocation density of character θ at location $\vec{r}$. Thus for a single dislocation *i* as shown in FIG. 2(a), the ϱ-field may be defined as:

$$\varrho_i(\vec{r},\theta) = \frac{\delta(r_i')}{b}\frac{\delta(\theta_i')}{2\pi} \tag{20}$$

where r_i' is the shortest distance of the dislocation from the field point $\vec{r}$, $\theta_i' = \theta - \theta_i$ with θ_i being the angular character of the dislocation at the point $\vec{r}_i$ which is nearest to the field point $\vec{r}$, and $\delta(x)$ is a delta-like function of a scalar variable *x*. Like eqn. (11), eqn. (20) says that ϱ_i is zero everywhere on the slip plane except when the field point $\vec{r}$ is on the dislocation line, and when this is the case, ϱ_i will still be zero unless θ equals the local dislocation character θ_i. Thus, over the $(\vec{r},\theta)$ space, non-zero counts of ϱ_i register the locations and local characters of dislocation *i*.

The time-evolution of ϱ_i at given $(\vec{r},\theta)$ due to movement of the dislocation on the slip plane is given by differentiating eqn. (20) with respect to time at fixed $(\vec{r},\theta)$:

$$\dot{\varrho}_i|_{(\vec{r},\theta)} = \frac{\delta(\theta_i')}{2\pi b}\delta'(r_i')\frac{\partial r_i'}{\partial t} + \frac{\delta(r_i')}{2\pi b}\delta'(\theta_i')\frac{\partial \theta_i'}{\partial t} = \frac{\delta(\theta_i')}{2\pi b}\delta'(r_i')\frac{\partial r_i'}{\partial t} - \frac{\delta(r_i')}{2\pi b}\delta'(\theta_i')\dot{\theta}_i$$

By defining $v_i = -\partial r_i'/\partial t$ as the speed of approach of the dislocation towards $\vec{r}$ as before, this becomes

$$\dot{\varrho}_i(\vec{r},\theta) = -\underbrace{\frac{\delta(\theta_i')}{2\pi b}v_i\,\delta'(r_i')}_{approach} - \underbrace{\frac{\delta(r_i')}{2\pi b}\dot{\theta}_i\,\delta'(\theta_i')}_{tilting} \tag{21}$$

When there are many dislocations moving on the slip plane, the total dislocation-density function $\varrho(\vec{r},\theta)$, and its flux quantities $\langle\varrho v\rangle$ and $\langle\varrho v_\theta\rangle$ can be defined as the sum of contributions of $\varrho_i(\vec{r},\theta)$ in eqn. (20):

$$\varrho(\vec{r},\theta) = \sum_i \varrho_i(\vec{r},\theta) = \frac{1}{2\pi b}\sum_i \delta(r_i')\delta(\theta_i') \tag{22}$$

$$\langle\varrho v\rangle(\vec{r},\theta) = \sum_i v_i\,\varrho_i(\vec{r},\theta) = \frac{1}{2\pi b}\sum_i v_i\,\delta(r_i')\delta(\theta_i') \tag{23}$$

$$\langle\varrho v_\theta\rangle(\vec{r},\theta) = \sum_i \dot{\theta}_i\,\varrho_i(\vec{r},\theta) = \frac{1}{2\pi b}\sum_i \dot{\theta}_i\,\delta(r_i')\delta(\theta_i') \tag{24}$$

It should be noted that the summations in these equations do not cancel out the SSD contents, since, for example, a dislocation dipole at the same field point $\vec{r}$ would have the two members registered in two θ_i values separated by π apart in $\delta(\theta_i')$, and so their ϱ_i, $\langle\varrho v\rangle$, or $\langle\varrho v_\theta\rangle$ values do not cancel out. From eqns. (21) and (22), the evolution of $\varrho(\vec{r},\theta)$ is

$$\dot{\varrho} = -\underbrace{\sum_i\left[\frac{\delta(\theta_i')}{2\pi b}v_i\,\delta'(r_i')\right]}_{movement} - \underbrace{\sum_i\left[\frac{\delta(r_i')}{2\pi b}\dot{\theta}_i\,\delta'(\theta_i')\right]}_{tilting} \tag{25}$$

and again, there is a term due to movements of dislocations, and another term due to their tilting. Furthermore, it is not difficult to see that eqn. (25) corresponds well to eqn. (19). Formally, from eqn. (23),

$$\frac{\partial\langle\varrho v\rangle}{\partial r_{\hat{\theta}}} = \frac{1}{2\pi b}\sum_i \delta(\theta_i')\frac{\partial[v_i\,\delta(r_i')]}{\partial r_{\hat{\theta}}} = \frac{1}{2\pi b}\sum_i \delta(\theta_i')\,v_i\,\delta'(r_i') \tag{26}$$

Here, by virtue of the $\delta(\theta_i')$ selector, $\partial r_{\hat{\theta}}$ refers to a movement of the field point ($\vec{r}$ in FIG. 2(a)) along the $\hat{\theta} = \hat{n} \times \hat{\xi}_\theta$ or r_i' direction of those dislocations *i* when their θ_i at the points closest to $\vec{r}$ are equal to a given θ; the second step of eqn. (26) then follows from the fact that the velocities v_i of such dislocations *i* would not change as the field point $\vec{r}$ moves this way. Similarly, from eqn. (24),

$$\frac{\partial\langle \varrho v_\theta \rangle}{\partial \theta} = \sum_i \left[\frac{\delta(r_i')}{2\pi b} \dot{\theta}_i \frac{\partial \delta(\theta_i')}{\partial \theta}\right] = \sum_i \left[\frac{\delta(r_i')}{2\pi b} \dot{\theta}_i \delta'(\theta_i')\right] \quad (27)$$

since $\theta_i' = \theta - \theta_i$ and θ_i and $\dot{\theta}_i$ are independent of a change $\partial\theta$ in the character space of $\varrho(\vec{r}, \theta)$. Thus, with eqns. (26) and (27), eqn. (25) becomes

$$\dot{\varrho} = \underbrace{-\frac{\partial\langle \varrho v \rangle}{\partial r_{\hat{\theta}}}}_{movement} \underbrace{- \frac{\partial\langle \varrho v_\theta \rangle}{\partial \theta}}_{tilting} \quad (28)$$

which corresponds exactly to eqn. (19).

We also note that eqn. (19) can be written in the alternative form:

$$\dot{\varrho}(\vec{r}, \theta) = -\vec{\nabla}(\varrho v) \cdot \hat{\theta} - \frac{\partial(\varrho v_\theta)}{\partial \theta} \quad (29)$$

where $\vec{\nabla}(\varrho v) \cdot \hat{\theta}$ denotes the gradient of the flux ϱv along the positive circumferential direction $\hat{\theta}$ of a given dislocation character θ.

Compatibility with CDD

Hochrainer et al.'s CDD theory [4] advocates the importance of the dislocation curvature [3, 4] as a second field variable in addition to the density itself. Specifically, in CDD, the evolution equation of the dislocation density is:

$$\dot{\varrho} = -\vec{\nabla} \cdot (\varrho \vec{v}) - \frac{\partial(\varrho v_\theta)}{\partial \theta} + \varrho v k \quad (30)$$

where k is the dislocation curvature.

Here, we show that eqn. (30) can be recovered from eqn. (29). Consider a density of dislocations near a field point $\vec{r}$ with a local curvature k there, as shown in FIG. 5(a). Without loss of generality, choose the coordinate system to be cylindrical (r, ϕ) with origin at the center of the fitting circle to the dislocation density, and unit vectors $\hat{r}$ and $\hat{\phi}$ along the radial and circumferential directions respectively. In this case, the quantity $\vec{\nabla}(\varrho v) \cdot \hat{\theta}$ in eqn. (29), which is a function of $\vec{r}$ and θ, will be non-zero only when $\vec{r} = (r, \phi)$ falls on the curved dislocation, i.e. $r = 1/k$. Furthermore, we also have $\hat{\theta} = \hat{r}$, since the velocity direction of the dislocation $\hat{v}$ or $\hat{\theta}$ is simply along the radial direction $\hat{r}$ of the cylindrical coordinate (see eqn. (6) and FIG. 5(a)). The non-zero value of $\vec{\nabla}(\varrho v) \cdot \hat{\theta}$ in eqn. (29) can therefore be expressed as

$$\vec{\nabla}(\varrho v) \cdot \hat{\theta} = \vec{\nabla}(\varrho v) \cdot \hat{r} = \vec{\nabla} \cdot (\varrho v \hat{r}) - (\varrho v)\, \vec{\nabla} \cdot \hat{r} = \vec{\nabla} \cdot (\varrho \vec{v}) - (\varrho v)\, \vec{\nabla} \cdot \hat{r} \quad (31)$$

in which,

$$\vec{\nabla}\cdot\hat{r} = \hat{r}\cdot(\partial\hat{r}/\partial r) + \left(\hat{\phi}/r\right)\cdot(\partial\hat{r}/\partial\phi)\big|_{r=1/k} = \left(\hat{\phi}/r\right)\cdot\hat{\phi}\big|_{r=1/k} = k$$

Eqn. (31) therefore gives $\vec{\nabla}(\varrho v)\cdot\hat{\theta} = \vec{\nabla}\cdot(\varrho\vec{v}) - \varrho v k$ and on substituting back to eqn. (29), eqn. (30) of the CDD theory is recovered.

Although the CDD eqn. (30) is compatible with the present eqn. (29), in the former, the dislocation density ϱ and curvature k are coupled variables solvable only with a simultaneous evolution equation for the curvature [3]. However, in eqn. (29), only the variable ϱ is involved which can be solved from that equation alone.

To further see that the curvature-generation term in the CDD is already embodied in eqn. (29), consider a simple example where an infinite series of concentric loops uniformly distributed along r are all expanding from the origin at the same speed (FIG. 5(b)). As such loops move past a fan-shaped control volume as shown in FIG. 5(b), the averaged dislocation density ρ, i.e. number of dislocations threading unit area perpendicular to the dislocation line (c.f. eqns. (1) and (2)), is a constant function of r, but since the arc length at $r + dr$ is longer than that at r, the total line length of dislocations arriving at the $(r + dr)$ boundary of the fan-shaped control volume is longer than that at r. Therefore, in the CDD eqn. (30), $\vec{\nabla}\cdot(\rho\vec{v}) > 0$, but since ρ is constant inside the control volume, the generation term $\rho v k$ has to be there to compensate. Alternatively, the fact that $\dot{\rho} = 0$ over the slip plane (except at the origin) can be embodied in a much simpler way by considering 1D flux divergence $\vec{\nabla}(\varrho v)\cdot\hat{\theta}$ along the $\vec{v}$ or $\hat{\theta}$ direction of the dislocations as in eqn. (29). Thus, in FIG. 5(b), if we count the arrival and departure of dislocations along any 1D radial direction, rather than across the 2D fan-shaped control volume shown, then the ρ sampled at r would be the same as that sampled at $r + dr$, and so $\partial(\rho v)/\partial r = \vec{\nabla}(\varrho v)\cdot\hat{\theta} = 0$, leaving no need for an extra generation term even though there is dislocation curvature.

Discussion and Conclusion

To summarize, in this work we have shown that an evolution equation for the dislocation character-specific density $\varrho(\vec{r},\theta)$ is eqn. (29), i.e.

$$\dot{\varrho}(\vec{r},\theta) = \underbrace{-\vec{\nabla}(\varrho v)\cdot\hat{\theta}}_{movement} \underbrace{- \frac{\partial(\varrho\, v_\theta)}{\partial\theta}}_{tilting} \tag{29}$$

Here, v is the dislocation velocity, v_θ the rotational speed of the dislocation, and $\hat{\theta}$ is the unit vector along the circumferential direction in the positive sense of θ on the slip plane. To close the problem, the dislocation velocity v needs to be evaluated from a known or assumed velocity law involving the effective glide stress which is the net of the applied stress, Peierls stress and elastic interactions between dislocation densities in the system [7]. Once the v-field is known, the rotational velocity can be evaluated as $v_\theta = dv/d\xi_\theta$ where ξ_θ is the dislocation line direction for a given character θ. Eqn. (29) describes the evolution of dislocation density of each dislocation character

θ, and hence it is much more comprehensive than eqn. (4) which is for the GNDs only, or Acharya and Roy's eqn. (10) [8] in which the evolution of the SSD term $\boldsymbol{L^p}$ is not exactly known. Compared to the CDD [4], eqn. (29) does not involve the dislocation curvature as a coupled variable. Eqn. (29) is also very simple to understand – the first term describes the coming and going of dislocations of the given dislocation character to and from the field point $\vec{r}$ along the dislocation velocity direction which is $\hat{\theta}$, while the second term describes the tilting of the dislocations away from the given dislocation character. Eqn. (29) is fully consistent with both Acharya's eqn. (5) and the CDD theory in eqn. (30), and so through it, the latter two theories are also shown to be compatible with each other. Future work should focus on numerically implementing eqn. (29) for the computation of real dislocation dynamics problems.

Acknowledgment

The work described in this paper is supported by Kingboard Endowed Professorship in Materials Engineering and Seed Fund for Basic Research (Project code: 201411159129) at the University of Hong Kong.

References

1. A. Acharya: A model of crystal plasticity based on the theory of continuously distributed dislocations. *J. Mech. Phys. Solids* **49**, 761 (2001).
2. A. El-Azab: Statistical mechanics treatment of the evolution of dislocation distributions in single crystals. *Phys. Rev.* **B 61**, 11956 (2000).
3. R. Sedláček, J. Kratochvil and E. Werner: The importance of being curved: bowing dislocations in a continuum description. *Philos. Mag.* **83**, 3735 (2003).
4. T. Hochrainer, M. Zaiser and P. Gumbsch: A three-dimensional continuum theory of dislocation systems: kinematics and mean-field formulation. *Philos. Mag.* **87**, 1261 (2007).
5. J.F. Nye: Some geometrical relations in dislocated crystals. *Acta Metal.* **1**, 153 (1953).
6. E. Kröner: *Kontinuumstheorie der Versetzungen und Eigenspannungen*. Berlin, Springer (1958).
7. H.S. Leung and A.H.W. Ngan: Dislocation-density function dynamics – An all-dislocation, full-dynamics approach for modeling intensive dislocation structures. *J. Mech. Phys. Solids* **91**, 172 (2016).
8. A. Acharya and A. Roy: Size effects and idealized dislocation microstructure at small scales: Predictions of a phenomenological mode of mesoscopic field dislocation mechanics: Part I. *J. Mech. Phys. Solids* **54**, 1687 (2006).
9. V. Taupin, S. Varadhan, C. Fressengeas and A.J. Beaudoin: Directionality of yield point in strain-aged steels: The role of polar dislocations. *Acta Mater.* **56**, 3002 (2008).

Figure Captions

FIG. 1 – Area density of dislocations on a slip plane

FIG. 2 – (a) Discrete dislocation i on slip plane (plane of this paper). A general field point $\vec{r}$ is at perpendicular (shortest) distance r_i' from the dislocation line. $\vec{r}_i$ is the point on the dislocation line that is nearest to the field point $\vec{r}$. Slip plane normal $\hat{n} = \hat{s} \times \hat{e}$ (i.e. pointing out of the plane of paper). (b) Displacing the field point by ∂x_2 along the local dislocation direction $\hat{\xi}_i$ results in change in r_i' by $\partial r_i'$ as shown.

FIG. 3 – A dislocation approaching a field point $\vec{r}$ with speed v_i, causing the dislocation density there to increase at a rate of $\dot{\rho}_i$.

FIG. 4 – Polar plot of the dislocation density ϱ at a given field point $\vec{r}$, showing the dislocation character (θ) dependence of the density.

FIG. 5 – (a) A density of dislocations (solid curve) at field point $\vec{r}$ with local curvature k moving with velocity $\vec{v}$. (b) Uniform distribution of concentric loops expanding at the same speed.

Figures

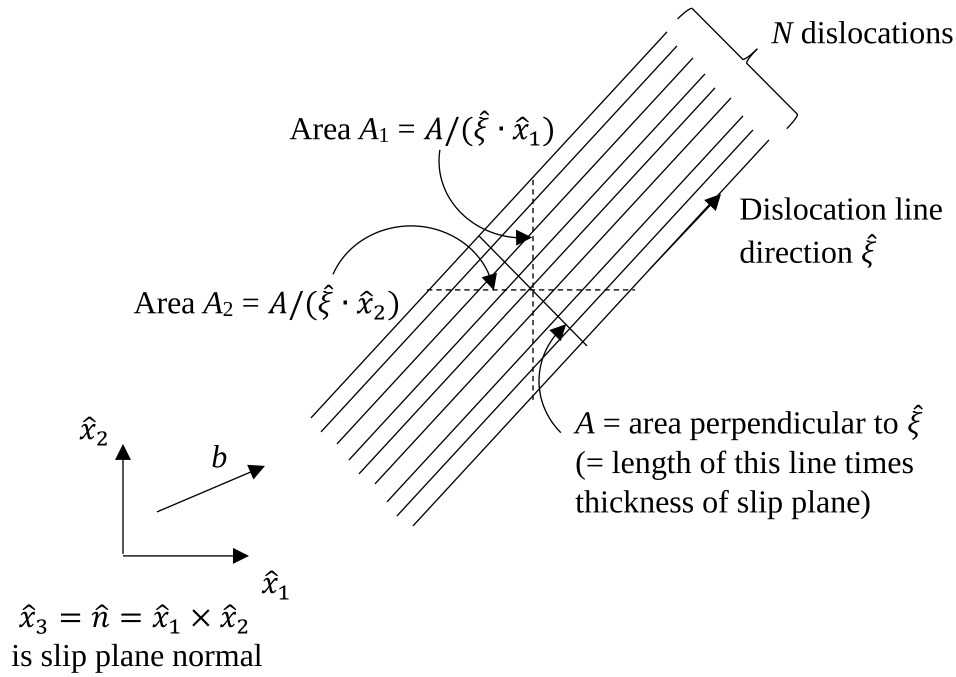
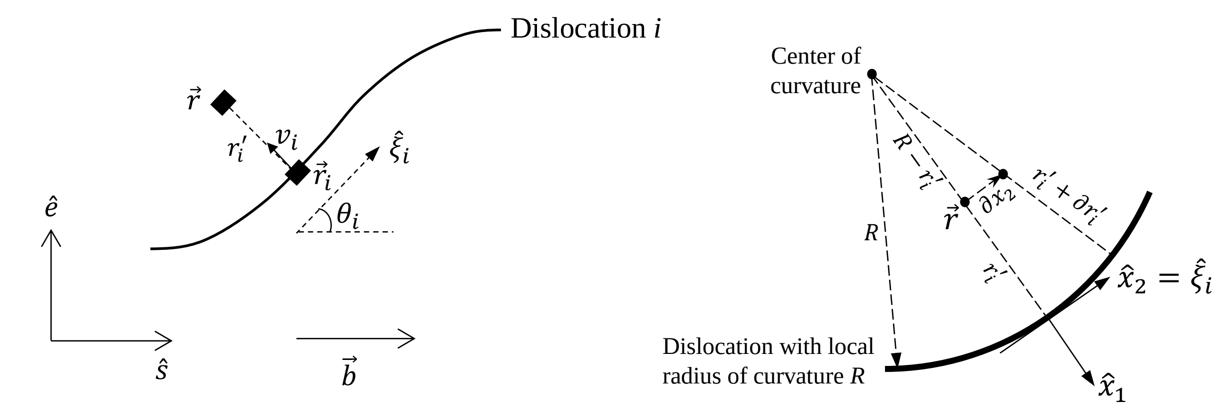


FIG. 1 – Area density of dislocations on a slip plane



(a) (b)

FIG. 2 – (a) Discrete dislocation i on slip plane (plane of this paper). A general field point $\vec{r}$ is at perpendicular (shortest) distance r_i' from the dislocation line. $\vec{r}_i$ is the point on the dislocation line that is nearest to the field point $\vec{r}$. Slip plane normal $\hat{n} = \hat{s} \times \hat{e}$ (i.e. pointing out of the plane of paper). (b) Displacing the field point by ∂x_2 along the local dislocation direction $\hat{\xi}_i$ results in change in r_i' by $\partial r_i'$ as shown.

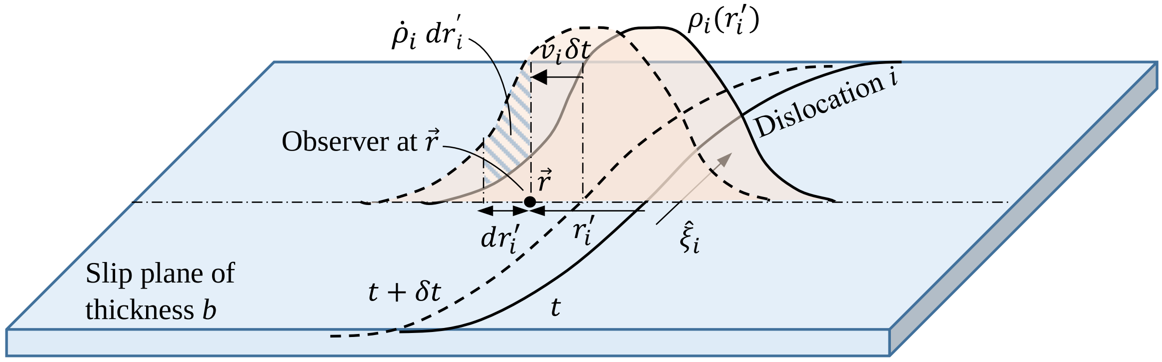


FIG. 3 – A dislocation approaching a field point $\vec{r}$ with speed v_i, causing the dislocation density there to increase at a rate of $\dot{\rho}_i$.

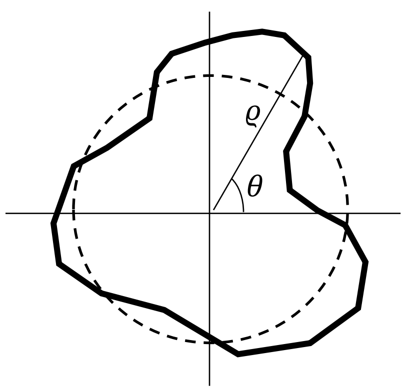


FIG. 4 – Polar plot of the dislocation density ϱ at a given field point $\vec{r}$, showing the dislocation character (θ) dependence of the density.

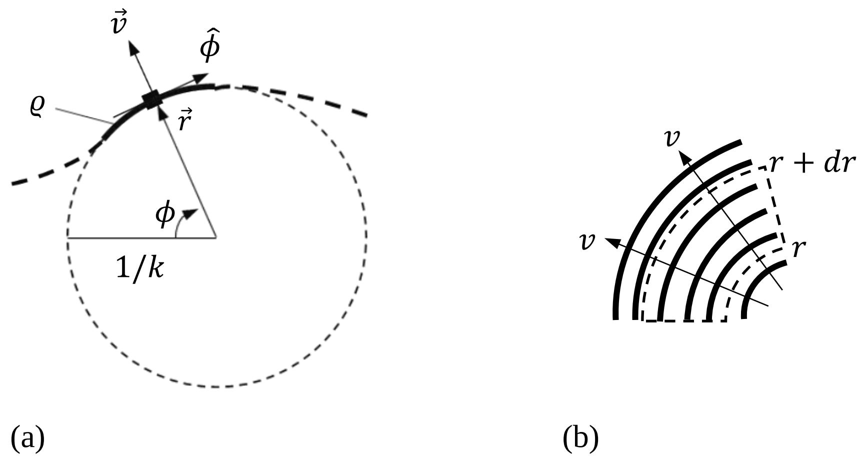


FIG. 5 – (a) A density of dislocations (solid curve) at field point $\vec{r}$ with local curvature k moving with velocity $\vec{v}$. (b) Uniform distribution of concentric loops expanding at the same speed.