Electric Field-Induced Forces upon Dislocations and Intrinsic Electric Interaction between Dislocations

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Dislocations and dislocation dynamics are the cores of material plasticity. In this work, we focus on and explore electric forces caused by external electric field upon dislocations and intrinsic electric forces between dislocations. Here we found that there exist a threshold electric field above which the electric field-induced force can enable dislocations glide and to one's surprise, being subject to the identical electric field, some dislocations move in one direction but others move reversely, which are in agreement with experimental observations and may be the microscopic physical mechanism of electroplasticity. Besides the classical known mechanic force, an important intrinsic electric force exists between dislocations, which is uncovered here for the first time and has been neglected since discovery of dislocations. The electric forces are short-range and apparent when the distance between dislocations is only several nanometers. These findings maybe assist people in understanding correlated physical phenomena, for instance, eletroplasticity, understanding actual underlying physics of plastic deformations and designing next-generation nano-devices.

1. Introduction

Dislocations are a primary crystalline plastic mechanism and dominate plastic behaviors of crystalline materials. Electronic properties of dislocations are of interest and vital importance, because dislocations are found to move under external electric field [1], meaning that the electric field may affect the plastic behaviors of crystalline materials, e.g. electroplasticity. They usually detrimentally reduce function of semiconductor-based devices [2], indicating that understanding electronic properties of dislocations is a key for next-generation nano-devices.

To explore electronic properties of dislocations, several experimental methods have been developed and utilized, for example, electron-beam-induced current (EBIC) of dislocations [3, 4], electrical conductivity of nano-contact semiconductor wafer with dislocations [5], electrical conductivity of dislocation-stored thin films [6], electrical voltage during dislocation-based plastic deformation [7], motion of low-angle grain boundaries constructed by edge dislocations under external electric field [8] and so on.

In the theoretical respect, electronic properties of dislocation were intensively investigated in terms of various methods. In the vicinity of an edge dislocation, an electrostatic potential was believed to exist for keeping the electronic conduction band uniform, and was used to calculate increased resistance of cold-worked copper [9]. An individual edge dislocation was thought to cause electron charge redistribution and result in electric interaction between a dislocation and a solute atom in metals [10]. Electronic structure of a dislocation was studied by virtue of a one-dimensional quantum wire model, and may the origin of some interesting electronic phenomena such as two-dimensional electron gas on dislocation network [11].

However, electronic properties of dislocations, especially electric force between dislocations and external electric field-induced electric force acting on dislocations, which may be the key for people understanding eletroplasticity, performances of nano-devices and real plastic deformations of crystalline materials, is still challenging due to lacking in knowledge on electric field surrounding dislocations.

In this work, we reveal an intrinsic electric field around a single dislocation, and give the electric force on dislocations induced by an external electric field as well as an intrinsic electric force between dislocations, which may help people re-understand dislocations.

2. Electric force on dislocations

Experimental observations on electroplasticity show that when mechanical plasticity happens for a material, flow stress is usually reduced noticeably by an applied electric field [12]. It is attributed to enhanced dislocation mobility, which arise from an electric field applying a driving force on dislocations [13, 14], however, its physical origin is unclear. In this part, the microscopic mechanism of electric field effect on dislocation motions is the concerns.

2.1 Electric force for an edge dislocation

Consider an individual edge dislocation in a simple cubic lattice. By means of the known stress field [15], strain field and *Yuheng Zhang Equation* [16], *i.e.* $q\vec{E} = \nabla E_F$, the electric field surrounding an edge dislocation is given by

$\vec{E}_1 = \frac{1}{q}\left(\frac{\delta E_F}{\delta \xi_{xx}} \nabla \xi_{xx} + \frac{\delta E_F}{\delta \xi_{yy}} \nabla \xi_{yy} + \frac{\delta E_F}{\delta \xi_{zz}} \nabla \xi_{zz} + \frac{\delta E_F}{\delta \xi_{xy}} \nabla \xi_{xy} + \frac{\delta E_F}{\delta \xi_{yx}} \nabla \xi_{yx} \right)$, where E_F is Fermi surface energy, namely, Fermi level, q is electron charge, $\overrightarrow{E_1}$ is electric field around an edge dislocation, ξ_{xx}, ξ_{yy}, ξ_{zz} and ξ_{xy} are strains. Due to the symmetry of cubic lattice,

$$V\frac{\delta E_F}{\delta V} = \frac{\delta E_F}{\delta \xi_{xx}} = \frac{\delta E_F}{\delta \xi_{yy}} = \frac{\delta E_F}{\delta \xi_{zz}};\quad \frac{\delta E_F}{\delta \xi} = \frac{\delta E_F}{\delta \xi_{xy}} = \frac{\delta E_F}{\delta \xi_{yx}} = \frac{\delta E_F}{\delta \xi_{xz}} = \frac{\delta E_F}{\delta \xi_{zx}} = \frac{\delta E_F}{\delta \xi_{yz}} = \frac{\delta E_F}{\delta \xi_{zy}}$$

$$\vec{E}_1 = \frac{mb_e}{2\pi(1-\nu)}\left[\frac{2xy}{\left(x^2+y^2\right)^2}\vec{x} + \frac{y^2-x^2}{\left(x^2+y^2\right)^2}\vec{y} \right] - \frac{nb_e}{2\pi(1-\nu)}\left[\frac{\left(x^2+y^2\right)^2 - 8x^2y^2}{\left(x^2+y^2\right)^3}\vec{x} + \frac{2xy\left(3x^2-y^2\right)}{\left(x^2+y^2\right)^3}\vec{y} \right] \quad (1)$$

where parameters m, n are $m = \frac{V}{q}\frac{\delta E_F}{\delta V}\left(1-2\nu\right)$ and $n = \frac{1}{q}\frac{\delta E_F}{\delta \xi}$, V, ν denotes unit volume and Poisson's ration, respectively, ξ stands for shear strain, b_e is Burgers vector of the edge dislocation. If an external electric field $\vec{E}_2$ was applied, $\vec{E}_2 = E_0\left(cos\psi\ \vec{x} + sin\psi\ \vec{y}\right)$ (E_0 is magnitude of the external field and ψ is the angle between Burgers vector and electric field), the total electric energy W is $W = W_1 + W_2 + W_{12}$, where W_1 and W_2 are electric energy of the dislocation and external field, W_{12} is the interconnection energy.

$$W_{12} = \frac{\varepsilon_0 \varepsilon m L b_e E_0}{4\left(1-\nu\right)}\left[n\,cos\left(\psi - 4\varphi\right) + 2n\,sin\psi\,sin\,2\varphi - 2m\,sin\left(\psi - 2\varphi\right) \right] \quad (2)$$

where ε_0 is vacuum dielectric permittivity, ε is relative dielectric permittivity, L is the dislocation length, φ is the polar angle of dislocation. For many materials, magnitude of parameter m may be much larger than n. So, if the external field is parallel to the Burgers vector, i.e., ψ=0, the electric energy is $W_{12} \approx \frac{\varepsilon_0 \varepsilon m L b_e E_0}{2\left(1-\nu\right)} sin\,2\varphi$. It is easily seen that when m>0, this energy is the smallest at polar angles 3π/4 and 7π/4, meaning dislocations (1) (in red color) stay in the most stable state in the external electric field, as is shown in Figure 1(a). But at polar angles π/4 and 5π/4, W_{12} is the highest, indicating dislocations (2) (in blue color) may undergo an electric force pointing to dislocations (1) as shown in Figure 1(a). The electric force F per unit length may approximate

$$F = \frac{\varepsilon_0 \varepsilon m b_e E_0}{(1-\nu) r_0} \cos 2\varphi \sin \varphi \tag{3}$$

where r_0 is distance of dislocation away from the center axis of crystalline grain. At some conditions, e.g. high temperatures and large external electric field, the electric force may exceed Peierls-Nabarro stress [15] and enables edge dislocations glide. So a threshold electric field E_c exists above which the edge dislocations can be driven to overcome motion barriers and glide,

$$E_{th} = \frac{2\mu r_0}{\varepsilon_0 \varepsilon m} \frac{exp\left[-2\pi a / b_e (1-\nu)\right]}{\cos 2\varphi \sin \varphi} \tag{4}$$

where μ is shear modulus, a is crystalline lattice parameter. This threshold field strongly depends on the distance r_0, relative dielectric permittivity ε and polar angle of this edge dislocation.

If the Burgers vector is perpendicular to the electric field, i.e., $\psi=\pi/2$, the interconnection energy is $W_{12} = -\frac{\varepsilon_0 \varepsilon m L b_e E_0}{2(1-\nu)} \cos 2\varphi$. If parameter m is also positive, W_{12} is the lowest at polar angles 0 and π, demonstrating that dislocations (1) are the most stable, but at polar angles π/2 and 3π/2 W_{12} is the largest, suggesting an electric force exerting on these dislocations, as is shown in Figure 1(b). Likely, its strength per unit length may be

$$F = \frac{\varepsilon_0 \varepsilon m b_e E_0}{(1-\nu) r_0} \sin 2\varphi \sin\varphi \tag{5}$$

Also, a corresponding threshold electric field E_{th} exists and it is

$$E_{th} = \frac{2\mu r_0}{\varepsilon_0 \varepsilon m} \frac{\exp\left[-2\pi a / b_e (1-\nu)\right]}{\sin 2\varphi \sin\varphi} \tag{6}$$

For many crystalline materials, the threshold fields at different conditions may be in the range $10^4 \sim 10^6$ V/m, and it may decrease with increasing temperatures because of material softening. These points were verified by electric field-driving motion of small angle-tilt grain boundaries constructed by array of edge dislocations [8]. Furthermore, according to the expressions of electric forces in the above two cases, the force are positive in some polar angle zones but negative in other angle zones. Therefore, under electric field, some dislocations are expected to glide parallel to the electric field, but some other dislocations are anticipated to move reversely, which is indeed the experimental observations that majority of dislocations move against the field but a large proportion still move in the field direction in sodium chloride [17, 18].

Edge dislocations can be driven to move by an electric field, but against numerous previous investigations on debated charges of edge dislocation [17, 19, 20, 21, 22], here it is found and argued that dislocations do not carry net charges actually, so that mobile edge dislocation themselves do not contribute to electrical conductivity.

2.2 Electric force for a screw dislocation

Let us move to the case of screw dislocation in simple cubic lattice. Also according to *Yuheng Zhang Equation* [16] and strain field of a screw dislocation [15], the induced electric field is obtained

$$\vec{E}_1 = \frac{nb_s}{2\pi}\left[\frac{y^2 - x^2 + 2xy}{\left(x^2 + y^2\right)^2}\vec{x} + \frac{y^2 - x^2 - 2xy}{\left(x^2 + y^2\right)^2}\vec{y}\right] \tag{7}$$

Due to rotation symmetry of screw dislocation in simple cubic lattice, the interconnection energy under the external electric field $\vec{E}_2 = E_0\left(cos\psi\ \vec{x} + sin\psi\ \vec{y}\right)$ is

$$W_{12} = -\frac{\varepsilon_0 \varepsilon n L b_s E_0}{\sqrt{2}} sin\left(\psi + \frac{\pi}{4}\right) \tag{8}$$

In the case of positive parameter n, this energy is the smallest at angle π/4, meaning that dislocations (1) (in red color) stay in the most stable state in the external electric field. But at angle 5π/4, W_{12} is the largest, indicating dislocations (2) (in blue color) may undergo an electric force. The strength of electric force per unit length may be

$$F = \frac{\varepsilon_0 \varepsilon n b_s E_0}{\sqrt{2} r_0} cos\left(\psi + \frac{\pi}{4}\right) \tag{9}$$

and its direction is tangentially pointing to dislocations (1) shown by the arrows in Figure 2. This force sensitively relies on the angle and distance from grain center axis, and may drive some dislocations into zones of dislocations (1), thereby forming dense zones and sparse zones of screw dislocations. If the sign of parameter n or Burgers vector possess a negative value, the interconnection energy and the electric force may also be reversed.

Interestingly, like edge dislocations, screw dislocations can be driven to move by an external electric field, but they do not carry net charges as well. So their motions also do not contribute to electrical conductivity of materials.

In the above quantitative analysis, only considered is the stain field of a dislocation, and its image dislocation and grain boundary relaxation effect on the strains and electric field in the grain is ignored. More accurately, their effects should be taken into account.

3. Electric interactions between dislocations

As far as is known, dislocation dynamics is the most concerned in the realm of material plasticity. For plastic deformations of materials, most researchers only consider mechanic interaction between dislocations but neglect another vital interaction, namely, intrinsic electric interaction between dislocations. In the following part, we will reveal this electric interaction.

3.1 Electronic interaction between two parallel edge dislocations

The electric field around an individual edge dislocation could be written as $\vec{E}=\frac{b_e}{2\pi(1-\nu)}(\lambda\vec{x}+k\vec{y})$, where parameters $\lambda = m\frac{2xy}{\left(x^2+y^2\right)^2} - n\frac{\left(x^2+y^2\right)^2-8x^2y^2}{\left(x^2+y^2\right)^3}$ and $k = m\frac{y^2-x^2}{\left(x^2+y^2\right)^2} - n\frac{2xy\left(3x^2-y^2\right)}{\left(x^2+y^2\right)^3}$. For most materials, the relation between parameters may hold $m >> n$, so the electric interaction energy between two parallel edge dislocations follows

$$W_{12} \approx \frac{\varepsilon_0 \varepsilon m^2 L}{4\pi(1-\nu)^2}\frac{\vec{b}_{e1}\cdot\vec{b}_{e2}}{r^2} \tag{10}$$

where r is the distance between the two dislocations and L is dislocation length, b_{e1} and b_{e2} are Burgers vectors of the two edge dislocations, respectively. Thus the related electric force per unit length is

$$F = \frac{\varepsilon_0 \varepsilon m^2}{2\pi(1-\nu)^2}\frac{\vec{b}_{e1}\cdot\vec{b}_{e2}}{r^3} \tag{11}$$

This force sensitively depends on parameter m and relative dielectric constant. According to Equation (11), when the two Burgers vector are parallel, the force is repulsive; and when they are antiparallel to each other, the force is attractive. The electric force may be a short-range force and could be ignored at large distance, because it decreases more quickly than elastic stress between edge dislocations. Of noted is that this electric force should be taken into account once the two dislocations are neighboring, e.g. at a distance smaller than 5 nm. So when dislocation density is very high, in other words, very small average distances among dislocations, both electric force and mechanic stresses between dislocations must be considered for dislocation motions and related plastic deformations.

3.2 Electric interaction between two parallel screw dislocations

Like the previous treatment, the electric force between two parallel screw dislocations may be derived in terms of electric interaction energy. Based on elastic strain field [15] and *Yuheng zhang Equation* [16], the electric interaction energy for dislocations may be given by

$$W_{12} \approx \frac{\varepsilon_0 \varepsilon n^2 L}{\pi} \frac{\vec{b}_{s1} \cdot \vec{b}_{s2}}{r^2} \tag{12}$$

where b_{s1} and b_{s2} are Burgers vectors of the two screw dislocations. L is length of screw dislocations , r is distance between two dislocations. So the electric force between two parallel screw dislocations of unit length at a distance r is

$$F \approx \frac{2\varepsilon_0 \varepsilon n^2}{\pi} \frac{\vec{b}_{s1} \cdot \vec{b}_{s2}}{r^3} \tag{13}$$

Analogous to the situation of edge dislocations, electric force between screw dislocation decreases rapidly with distance and may be ignored for distances larger than 100 nm at room temperature. However, if the distance is only several nanometers, the electric force may be evident, which can affect plastic deformations of materials.

3.3 Corrections for image forces of dislocations

The image force of a dislocation near a planar grain boundary may be regarded as the interaction between the dislocation and its image dislocation. The classical image force of dislocations only takes into account the mechanic force and neglect their electric force [15, 23]. So the image forces should be corrected and related corrections for an edge dislocation and a screw dislocation per unit length are

$$F = -\frac{\mu b_e^2}{4\pi(1-\nu)l} - \frac{\varepsilon_0 \varepsilon m^2}{16\pi(1-\nu)^2} \frac{b_e^2}{l^3} \tag{14}$$

$$F = -\frac{\mu b_s^2}{4\pi l} - \frac{\varepsilon_0 \varepsilon n^2}{4\pi} \frac{b_s^2}{l^3} \tag{15}$$

where l is the distance from planar grain boundary, b_e and b_s are Burgers vectors of the edge dislocation and image dislocation, as is shown in Figure 3. The first term is the mechanic force [15, 23] and the second term is the electric force. The electric forces are also attractive and are in the same direction as the mechanic forces. As pointed out previously, for many crystalline materials, only when the distance $2l$ is several nanometers, may the corrected electric forces be of paramount importance.

4. Conclusion

In this work, we mainly study external electric field-induced electric forces upon dislocations and the intrinsic electric forces between dislocations. A threshold electric field exist, above which the electric field-induced force can enable dislocations glide, and interestingly, some dislocations move in one direction but others move reversely, as may be the underlying physical origin of electroplasticity and rules of designing next-generation nano-devices. On the other hand, besides the classical known mechanic force, there exists an important intrinsic electric force between dislocations, which is uncovered here first and has been neglected for more than half a century. The electric forces are short-range forces and are evident when the distance between dislocations is only several nanometers. It is anticipated to play a key role and help people reexamine related plastic deformations of materials.

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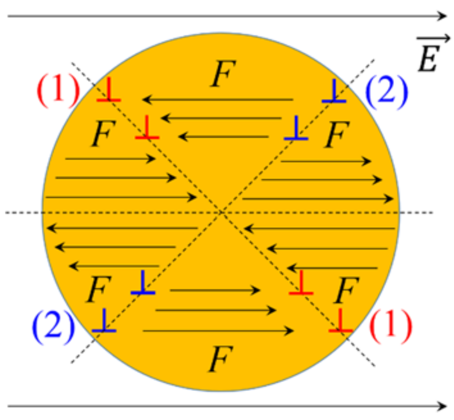
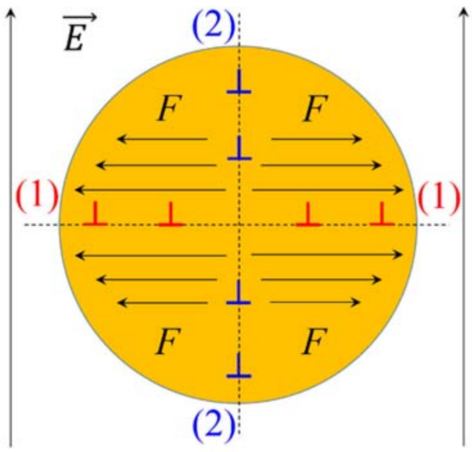


(a) ψ=0



(b) ψ=π/2

Figure 1 edge dislocations in a crystalline grain under an external electric field $\overrightarrow{E}$ which is parallel (a) to and perpendicular (b) to the Burgers vector. If the parameter $m = \frac{V}{q}\frac{\delta E_F}{\delta V}(1-2\nu)$ is positive, (a) interconnection energy of edge dislocations (1) (in red color) whose polar angle is 3π/4 and 7π/4 in the electric field are the smallest so that they are the most stable, but the interconnection energy of dislocations (2) (in blue color) whose polar angle is π/4 and 5π/4 is the largest; (b) electric energy of edge dislocations (1) (in red color) whose polar angle is 0 and π in the electric field are the smallest, however, the electric energy of dislocations (2) (in blue color) whose polar angle is π/2 and 3π/2 is the largest. Therefore, the dislocations per unit length may experience an electric force $F = \frac{\varepsilon_0 \varepsilon m b_e E_0}{(1-\nu) r_0} cos\, 2\varphi \, sin\, \varphi$ and $F = \frac{\varepsilon_0 \varepsilon m b_e E_0}{(1-\nu) r_0} sin\, 2\varphi \, sin\, \varphi$ for (a) and (b), respectively.

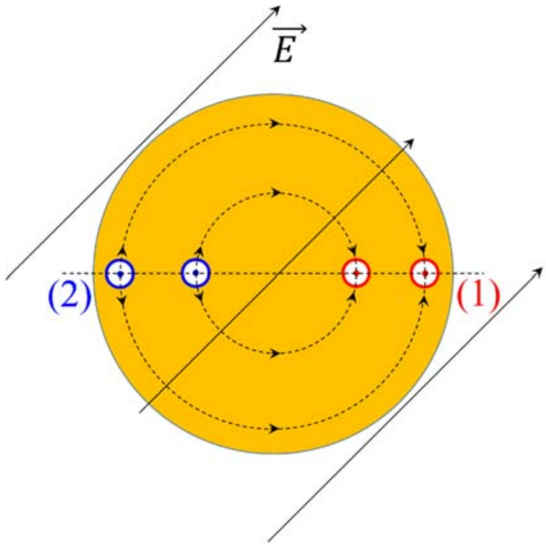


Figure 2 screw dislocations in a crystalline grain in an external electric field and the Burgers vector upwards through the paper. If the parameter $n = \frac{1}{q}\frac{\delta E_F}{\delta \xi}$ is positive, interconnection energy of screw dislocations (1) (in red color) in the electric field are the smallest and they are stay in the most stable state, but the interconnection energy of dislocations (2) (in blue color) is the largest, meaning that they may experience an electric force pointing to dislocations (1). Interconnection energy of dislocations (3) (in black color) is intermediate and approaches zero, may also undergo an electric force pointing to dislocations (1).

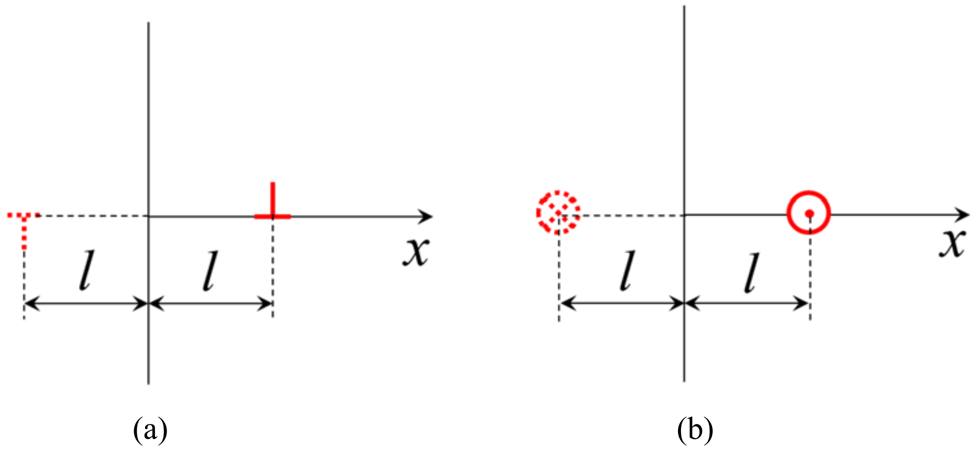


Figure 3 Dislocations near planar grain boundary and their image dislocations. (a) an edge dislocation (in red) and its image dislocation (in red) at a distance l away from grain boundary and their Burgers vectors at x axis; (b) a screw dislocation (in red) and its image dislocation (in red) at a distance l from grain boundary, and their Burgers vectors are directed perpendicularly out of the screen and into the screen, respectively.