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Exact solution of the generalized Peierls equation for arbitrary n-fold screw dislocation

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ABSTRACT

The exact solution of the generalized Peierls equation is presented and proved for arbitrary n-fold screw dislocation. The displacement field, stress field and the energy of the n-fold dislocation are also evaluated explicitly. It is found that the solution defined on each individual fold is given by the tail cut from the original Peierls solution. In viewpoint of energetics, a screw dislocation has a tendency to spread the distribution on all possible slip planes which are contained in the dislocation line zone. Based on the exact solution, the approximated solution of the improved Peierls equation is proposed for the modified γ-surface.

Introduction

In 1940s, Peierls put forward a famous equation and obtained the exact solution that can reveal the characteristic size of dislocations and predict the strength of materials (Peierls, 1940). The equation is generally named as Peierls equation and the related model is called Peierls model or Peierls–Nabarro (P-N) model (Hirth and Lothe, 1982; Nabarro, 1947). P-N model incorporated with the first-principles calculations is widely used to investigate dislocations in a variety of materials (Chen et al., 2015; Christian and Vitek, 1970; Dai et al., 2014; Lejček and Kroupa, 1976; Hirel et al., 2014; Hu and Wang, 2018; Joós et al., 1994; Liu et al., 2009; Ngan, 1995, 1997; Wang, 2002, 2015; Wang et al., 2014; Yan et al., 2004; Yao et al., 1999; Zhang et al., 1989; Zongrui et al., 2015).

A screw dislocation usually has more than one slip plane across the dislocation line. Hirsch firstly suggested that rather than planar core structure, the core of a screw dislocation distributes to several planes and displays multi-fold structure (Hirsch et al., 1960). This concept is largely confirmed by various numerical simulations and theoretical investigations (Dezerald et al., 2014; Duesbery and Vitek, 1998; Lejček and Kroupa, 1976; Hu and Wang, 2018; Ngan, 1995, 1997; Vitek and Paidar, 2008; Weinberger et al., 2013; Woodward and Rao, 2002; Zhang et al., 1989). Now, it is generally believed that screw dislocation in BCC lattice possesses a multi-fold core structure.

Dislocation is the source of the elastic field. Peierls model makes the elastic field theory becomes the first one that can determine the source structure in a self-consistent way. In the model, an elementary dislocation with the minimum Burgers vector is instructively viewed as a condensate of infinitesimal dislocations. The equilibrium structure results from balance between the expelling interaction and attracting interaction among the infinitesimal dislocations. It is recognized that the expelling interaction is identified with the self-energy, which is given in the elastic continuum theory of dislocations, and

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the attracting interaction is originated from the misfit energy, which is given by the generalized stacking-fault energy (γ-surface) proposed by Christian and Vitek (1970).

For a straight screw dislocation that lies along the z-axis, the dislocation structure can be described by a flux distribution $J(x, y)$ on the cross section. The total flux is the Burgers vector

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} J(x,y)dxdy = b.$$

For a n-fold dislocation, it is helpful to introduce fold distribution

$$J_s(x,y) = j_s(x_s)\delta(y_s)\theta(x_s),$$

where $\delta(x)$ is the Dirac-δ function, $\theta(x)$ is the Heaviside-θ function,

$$x_s = x\cos\alpha_s + y\sin\alpha_s, \qquad y_s = -x\sin\alpha_s + y\cos\alpha_s,$$

α_s is the angle between the orientation of the fold and the x-axis, $j_s(x)$ is the fold distribution that describes the dislocation distribution along the fold. Obviously, the flux distribution of a n-fold structure is simply given by summation

$$J(x,y) = \sum_{s=1}^{n} J_s(x,y) = \sum_{s=1}^{n} j_s(x_s)\delta(y_s)\theta(x_s). \tag{1}$$

As is well known, Hirth and Lothe (1982), the elastic interaction energy between two parallel dislocation lines b_1 and b_2 is

$$\varphi(r) = -\frac{\mu b_1 b_2}{2\pi}\ln\frac{r}{R},$$

where μ is the shear modulus (energy factor of a screw dislocation), r is the distance between two dislocations and R is the size of the bulk. The interaction energy (self-energy) of infinitesimal dislocations is given by,

$$U_i = -\frac{\mu}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} J(x,y)J(x',y')\ln\left|\frac{\sqrt{(x-x')^2+(y-y')^2}}{R}\right|dxdydx'dy' \times \frac{1}{2}, \tag{2}$$

where factor $\frac{1}{2}$ appears due to the double counting in the integration. For symmetric n-fold structure, $j_s(x) = j(x)$, the interaction energy is simplified as Hu and Wang (2018)

$$U_i = -\frac{n\mu}{4\pi}\int_0^{\infty}\int_0^{\infty} j(x)j(x')\ln\left|\frac{x^n - x'^n}{R^n}\right|dxdx'.$$

As pointed by Eshelby, the fold distribution is given by the derivative of the mismatch (disregistry) field

$$j(x) = \frac{du(x)}{dx}, \tag{3}$$

where the mismatch field $u(x)$ is defined by the local relative-displacement (Peierls, 1940; Wang, 2015). The density of misfit energy is a local function of the mismatch field. The misfit energy is

$$U_m = n\int_0^{\infty}\gamma(u)dx,$$

where $\gamma(u)$ is generally identified with the generalized stacking-fault energy (GSFE, or γ-surface) (Christian and Vitek, 1970). In the first approximation (Peierls, 1940),

$$\gamma(u) = \frac{\mu_\gamma b^2}{2\pi^2 d}\sin^2\frac{\pi u}{b},$$

where μ_γ is the effective shear modulus associated with the γ-surface. The total energy functional of a symmetric n-fold dislocation is

$$U = -\frac{n\mu}{4\pi}\int_0^{\infty}\int_0^{\infty} j(x)j(x')\ln\left|\frac{x^n - x'^n}{R^n}\right|dxdx' + \frac{n\mu_\gamma b^2}{2\pi^2 d}\int_0^{\infty}\sin^2\frac{\pi u}{b}dx. \tag{4}$$

The equation resulting from the minimum energy principle is

$$-\frac{\mu}{2\pi}\int_0^{\infty}\frac{nx^{n-1}}{x'^n - x^n}\frac{du}{dx}\bigg|_{x=x'}dx' = -\frac{\mu_\gamma b}{2\pi d}\sin\frac{2\pi u}{b}. \tag{5}$$

This equation is a generalization of the classical Peierls equation. For $n = 2$, it identifies with the classical Peierls equation (Peierls, 1940). For $n = 3$, it was obtained by Lejček and Kroupa (1976). For arbitrary n, it was firstly derived by Ngan using conformal mapping (Ngan, 1995, 1997). We refer this equation to as generalized Peierls equation.

The total Burgers vector equally distributes into n-fold for a symmetric n-fold dislocation and so each individual fold has Burgers vector

$$\int_0^{\infty} j(x)dx = u(\infty) - u(0) = \frac{b}{n}.$$