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Short Communication

Self-energy of dislocations and dislocation pileups

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ABSTRACT

A continuum model of dislocation pileups that takes the self-energy of dislocations into account is proposed. An analytical solution describing the distribution of dislocations in equilibrium is found from the energy minimization. Based on this solution we show (i) the existence of a critical threshold stress for the equilibrium of dislocations within a double pileup, and (ii) the existence of a non-linear regime in which the number of dislocations in a double pileup does not scale linearly with the resolved external shear stress, contrary to the classical double pileup model.

1. Introduction

In recent years there is a substantial amount of literature dealing with the dislocation pileups in crystals within the continuum approach (see, e.g., Berdichevsky & Le, 2007; Gurtin, 2002; Gurtin, Anand, & Lele, 2007; Kaluza & Le, 2011; Kochmann & Le, 2008a; 2008b; Le & Nguyen, 2012; 2013; Le & Sembiring, 2008a; 2008b; 2009; Ohno & Okumura, 2007 and the references therein). The proposed models turn out to be quite useful as they can predict the size effect for the yield stress, which agrees well with the experimental data (Ohno & Okumura, 2007) but however does not confirm the well-known empirical law formulated by Hall (1951) and Petch (1953). A traditional explanation of the Hall–Petch relation, based on the classical dislocation pileup model considered in Leibfried (1951), is that dislocation pile-ups serve to enhance the stress felt at grain boundaries. However, the Leibried's dislocation pileup model differs from the contemporary continuum models (Berdichevsky & Le, 2007; Kaluza & Le, 2011; Kochmann & Le, 2008a; 2008b; Le & Nguyen, 2012; 2013; Le & Sembiring, 2008a; 2008b; 2009; Ohno & Okumura, 2007) in two important aspects: firstly the absence of a threshold stress for dislocation nucleation, and secondly the absence of a finite-sized dislocation-free region. This is the motivation for us to reconsider the Leibfried's model in order to resolve this discrepancies.

Leibfried's one-dimensional theory of dislocation pileups is based on the force equilibrium: the Peach–Koehler resultant force acting on a dislocation produced by applied external stress and by other dislocations must vanish (Eshelby, Frank, & Nabarro, 1951; Leibfried, 1951). Within the continuum approximation one can deduce from here the well-known integral equation (Leibfried, 1951), provided the dislocation density is not zero. This equation need not be satisfied in a dislocation-free zone. In his now classical paper Leibfried (1951) mentioned that the natural way to find the stable equilibrium distribution of dislocations if such a zone occurs is to use the variational principle of minimum energy: among all admissible distributions of dislocations the true stable distribution minimizes energy of the crystal (cf. with the LEDS-hypothesis formulated in Hansen & Kuhlmann-Wilsdorf, 1986). To the best of the author's knowledge, the one-dimensional continuum model of dislocation pileups based on the energy minimization taking the self-energy of dislocations into account has not yet been proposed. The aim of this short

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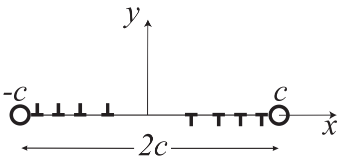

Fig. 1. Double pileup of edge dislocations.

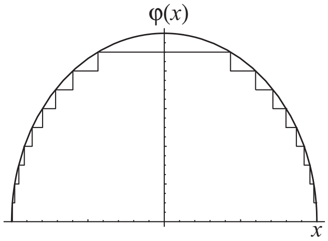

Fig. 2. Continuum approximation of the closure failure.

paper is to fill this gap. We start from the expression for the energy of crystal containing an array of dislocations which includes also the self-energy of dislocations. The self-energy density is proportional to the absolute value of the dislocation density, so this does not change the resultant force acting on the dislocation as well as the integral equation except the forces acting at the tails of the pileups. However, this self-energy influences the stable equilibrium distribution of dislocations essentially. We will show that the density of dislocations is identically zero if the applied stress is found below some critical value called the yield (or threshold) stress. Besides, the number of dislocations depends on the applied stress non-linearly, in contrast to the classical theory. The results of the proposed theory agree quite well with those of the continuum models of dislocation pileups obtained in Berdichevsky & Le (2007), Kaluza & Le (2011), Kochmann & Le (2008a; 2008b) and Le & Sembiring (2008a; 2008b; 2009). A continuum model of dislocation pile-ups taking into account the Frank-Read source proposed in Friedman & Chrzan (1998) (see also Chakravarthy & Curtin, 2010) leads to the similar results although it does not have the energetic structure.

In the next Section we present the continuum model of dislocation pileup accounting for the self-energy of dislocations. In Section 3 the energy minimization problem is solved and the related property of the solution is discussed. Section 4 shows the comparison between the theory and experiments. Finally, Section 5 concludes the paper.

2. Continuum model of dislocation pileup

Consider the plane strain problem of an infinite crystal which is uniformly loaded by a shear stress τ applied at infinity. Under this loading condition a linear array of equal number of positive and negative edge dislocations may occur on the slip line which is chosen to be the x-axis (see Fig. 1). The dislocation lines are parallel to the z-axis, while their Burgers vectors are directed along the x-axis. We assume that there are two obstacles (like two inclusions or grain boundaries) at $x = \pm c$ so that dislocations are confined to stay in the interval $L = (-c, c)$ of the x-axis. In the continuum limit we may replace the sum of many closure failures induced by dislocations in form of step functions by a smooth function $\varphi(x)$ (see Fig. 2). The obstacles impose the following constraints on this function

$$\varphi(\pm c) = 0. \tag{1}$$

Now we present the resultant inverse plastic distortion (Le, 2010) in the form

$$-\beta_{xy} = \varphi(x)\delta(y),$$

with $\delta(y)$ being the Dirac-delta function. Differentiating this equation with respect to x we obtain

$$-\beta_{xy,x} = \varphi'(x)\delta(y). \tag{2}$$

The interpretation of (2) is quite simple: if we integrate this equation over a circle C with the middle point at $x = -c$ and the radius $c + x$, then

$$-\int_C \beta_{xy,x}\, dxdy = -\int_{\partial C} \beta_{xy} dy = \int_{-c}^{x} \varphi'(\xi)\, d\xi = \varphi(x).$$

Thus, we get the closure failure of an amount $\varphi(x)$ which should be equal to the net Burgers vector of all dislocations within the interval $(-c, x)$. Denoting the dislocation density by $\rho(x)$, we get

$$\varphi(x) = b\int_{-c}^{x} \rho(\xi)\, d\xi \quad \Rightarrow \varphi'(x) = b\rho(x). \tag{3}$$