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ORIGINAL PAPER

V. L. Berdichevsky · V. G. Soutyrine

On the yield strength of periodic dislocation structures

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Abstract In his seminal paper of 1934, Taylor not only introduced the notion of dislocation, but also explained work hardening by dislocation interactions. To determine the critical shear stress needed to put dislocations in motion he considered a periodic set of edge dislocations with one positive and one negative dislocation in a cell. He found the critical stress to be of the form $\alpha_0\mu b/\epsilon$, where μ is shear modulus, b the interatomic distance, ϵ the cell size, α_0 some dimensionless constant. Since the dislocation density ρ in this problem is $2/\epsilon^2$, the critical stress can be written in the form of a relation of yield stress σ_Y and the dislocation density ρ, $\sigma_Y = \alpha\mu\sqrt{\rho}b$, $\alpha = \alpha_0/\sqrt{2}$. This formula is proved to be widely applicable and often referred to as Taylor's relation. We discuss in this paper whether the formula for critical stress, $\sigma_Y = \alpha_0\mu b/\epsilon$, yields Taylor's relation for a large number of edge dislocations in a periodic cell. This would be the case if the constant α_0 grows with the number of dislocations in a cell m as $\sqrt{m}$. Then, since $\rho = m/\epsilon^2$, Taylor's relation follows from the formula for the critical stress of periodic dislocation structures indeed. We give here an analysis of previously reported numerical simulations which indicates that α_0 appears to be finite as m increases. In other words, for 2D periodic dislocation ensembles, the strengthening coefficient α seems to be decaying as $1/\sqrt{m}$ and the proper relation for the yield strength of 2D periodic structures is $\sigma_Y = \alpha_0\mu b/\epsilon$. Thus, the yield strength depends on the cell size, and 2D periodic dislocation structures follow the similitude principle of cell structures rather than Taylor's glide resistance relation.

The first success of dislocation theory was an explanation of the physical origin of work hardening by G.I. Taylor [1]. In this seminal paper, Taylor not only introduced the notion of dislocation, but also associated work hardening with dislocation interactions. To find the critical shear stress needed to put dislocations in motion he considered a periodic set of dislocations with one positive and one negative dislocations in a cell. He found the critical stress to be of the form

$$\sigma_Y = \alpha_0\mu b/\epsilon, \tag{1}$$

where b is the interatomic distance, ϵ the cell size, α_0 some constant. For such a dislocation structure, the dislocation density ρ is $2/\epsilon^2$, and formula (1) can be written in the form of a relation of yield stress σ_Y and dislocation density ρ,

$$\sigma_Y = \alpha\mu\sqrt{\rho}b. \tag{2}$$

Formula (2) was widely supported by experimental observations and is often referred to as Taylor's relation [2,3]. Formula (2) was not written in Taylor's paper. By Mott's recollection included in Batchelor's memoir

V. L. Berdichevsky (✉)
Mechanical Engineering, Wayne State University, Detroit, MI 48202, USA
E-mail: vberd@eng.wayne.edu

V. G. Soutyrine
Sunnyvale, USA
https://www.linkedin.com/in/vladsoutyrine

[4], Taylor never returned to the subject. Perhaps, for the first time formula (2) was given by Bailey and Hirsch [5].

For two dislocations per cell, the strengthening coefficient α is equal to $\alpha_0/\sqrt{2}$. Total dislocation density ρ measured for some area ϵ^2 involves the number of dislocations m crossing this area: $\rho = m/\epsilon^2$. Therefore, strictly speaking, the derivation of (2) from (1) should be done for any number m of dislocations per cell. Formula (2) would follow from (1), if constant α_0 grows with the number of dislocations in a cell as $\sqrt{m}$. We give here an analysis of numerical simulations by Soutyrine et al. [6] which shows that this does not seem to occur, and, in fact, α_0 appears to be finite as m increases. In other words, formula (1) seems to be the proper relation for the yield strength of 2D periodic structures. One can interpret relation (1) as a "similitude principle" for 2D periodic structures (see a detailed discussion of the similitude principle given by Sauzay and Kubin [7]). Accordingly, plasticity of 2D periodic dislocation structures is similar to plasticity of dislocation cell structures.

The setting of numerical simulations in Ref. [6] is as follows. It was considered an unbounded plane covered by a periodic set of edge dislocations with the same slip plane. Let $\{x, y\}$ be Cartesian coordinates in the unbounded plane. The x-axis is directed along the Burgers vector. The x-component of the Burgers vector takes the values $\pm b$. It is convenient to scale the coordinates by the cell period ϵ and to use dimensionless coordinates $X = x/\epsilon$ and $Y = y/\epsilon$; in the basic cell, $|X| \leqslant 1/2, |Y| \leqslant 1/2$. The dislocation ensemble is neutral, i.e., the numbers of positive and negative dislocations are the same and equal to n, $m = 2n$. Polarization of the dislocation ensemble is characterized by the parameter

$$P = \frac{1}{m}\left(\sum_{i=1}^{n} X_i^+ - \sum_{i=1}^{n} X_i^-\right), \tag{3}$$

where X_i^+ and X_i^- are coordinates of positive and negative dislocations in the basic cell.

Polarization P can be chosen as one of coordinates of the dislocation ensemble. One more coordinate can be fixed due to transitional invariance of the system. Denote the remaining $m-2$ coordinates by ξ. For definiteness, we set $\sum X_i^+ + \sum X_i^- = 0$, and introduce ξ_i^+, ξ_i^- as

$$\xi_i^+ = X_i^+ - P, \quad \xi_i^- = X_i^- + P.$$

They obey two constraints:

$$\sum_{i=1}^{n} \xi_i^+ = 0, \quad \sum_{i=1}^{n} \xi_i^- = 0. \tag{4}$$

Equilibrium positions of the dislocation ensemble are stationary points over P, ξ of dimensionless energy [8]

$$\gamma(P, \xi) - \sigma P, \tag{5}$$

where ξ is the set of coordinates $\left\{\xi_1^+, \ldots, \xi_n^+, \xi_1^-, \ldots, \xi_n^-\right\}$, σ the dimensionless shear stress,

$$\sigma = \sigma_{xy}^{\infty}(1-\nu) \Big/ \frac{\mu b}{\epsilon}, \tag{6}$$

σ_{xy}^{∞} the shear stress applied at infinity, ν the Poisson coefficient. The function $\gamma(P, \xi)$ was found analytically, but its precise expression is not essential for what follows. It is only important that $\gamma(P, \xi)$ has a lot of local minima over ξ for a given P.

If an external stress σ is applied to a dislocation structure, dislocations slip into an equilibrium position, a local minimum of $\gamma(P, \xi)$ over ξ for a given P, determined by the equations

$$\frac{\partial \gamma(P, \xi)}{\partial \xi_i^+} = \lambda^+, \qquad \frac{\partial \gamma(P, \xi)}{\partial \xi_i^-} = \lambda^-. \tag{7}$$

Here λ^+, λ^- are Lagrange's multipliers for the constraints (4). In equilibrium, the external stress σ is balanced by the dislocation structure resistance, $\gamma_P = \partial\gamma(P, \xi)/\partial P$,

$$\frac{\partial \gamma(P, \xi)}{\partial P} = \sigma. \tag{8}$$

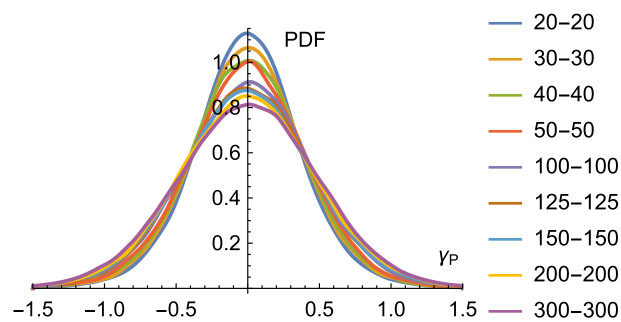

Fig. 1 Probability distribution of internal resistance γ_P of randomly cast neutral dislocation sets with different number of dislocations. In the legend, symbol "20-20" marks the dislocation ensembles with 20 positive and 20 negative dislocations in periodic cell; other legend notations are similar and show the number of dislocations in periodic cell. It is seen that there is no convergence when the number of dislocations increases

Equation (8) serves to find P for a given σ.

In a loading process, the current dislocation structure depends on the initial dislocation structure and the loading path. For a slow loading, the evolution is an intermittent process: It is a succession of slow deformations of the dislocation structure and fast slip avalanches. The slow parts consist of local equilibria, the solutions of Eqs. (7) and (8) [8].

For the Taylor case of 2 dislocations, γ is a periodic function of P only. The internal resistance γ_P is bounded, and, when σ exceeds the maximum value of the internal resistance, the plastic strain grows indefinitely. The maximum possible values of γ_P are different for each slow loading path and each initial dislocation structure. According to the Taylor picture of work hardening, the dimensionless yield strength σ_Y^* should be identified with maximum values of γ_P over all microstructures,

$$\sigma_Y^* = \max_{P,\check{\xi}} \frac{\partial \gamma \left(P, \check{\xi}\right)}{\partial P}, \tag{9}$$

where $\check{\xi}$ are stationary points of energy over ξ for fixed P.

In dimensional form, according to Eqs. (6) and (9), the yield strength is

$$\sigma_Y = \frac{\mu b}{(1-\nu)\,\epsilon}\sigma_Y^*. \tag{10}$$

So, to find the yield strength one has to determine σ_Y^* =maxγ_P. No means seem to exist to obtain the maximum possible value of γ_P analytically. One can try to get an upper bound for σ_Y^* by replacing the set of equilibrium dislocation structures with a much wider set of randomly and independently distributed dislocations. Then probability distribution of γ_P can be found by analytical methods developed in [9–12]. It turns out, however, that this does not yield a meaningful bound because the variance of γ_P grows with m. Numerical simulations of the probability density function (PDF) of γ_P for randomly placed dislocations are shown in Fig. 1 and support this result.

Another approach is to find numerically the probability distribution of γ_P for equilibrium dislocation structures. To this end, a neutral set of edge dislocations was cast in a periodic cell and then relaxed to equilibrium for a given P. There are two basic ways of relaxation. One is to solve dynamical equations for a given P, another one is to find local minima of $\gamma(P,\xi)$ over ξ. The second one was used in [6]. Surprisingly, in contrast to the case of randomly placed dislocations, the probability density functions of γ_P for equilibrium dislocation structures appear to be converging very fast to the limit distribution when the number of dislocations increases. The limit distribution is practically independent of P. It is shown in Fig. 2. As follows from Fig. 2, for an equilibrium structure, with overwhelming probability γ_P is a number in the interval $[0,\ 0.3]$, so $\sigma_Y^* \geq 0.3$. There are tiny tails of probability density functions which are not shown in Fig. 2; they go up to γ_P of order unity. In about 108,000 realizations used to obtain probability densities, the maximum value of γ_P observed was 1.5. Though numerical simulations cannot provide the exact value of σ_Y^*, σ_Y^* is likely of order unity. Much more details on statistical properties of equilibrium edge dislocation configurations can be found in [6,13–15], see also the reviews [16,17].

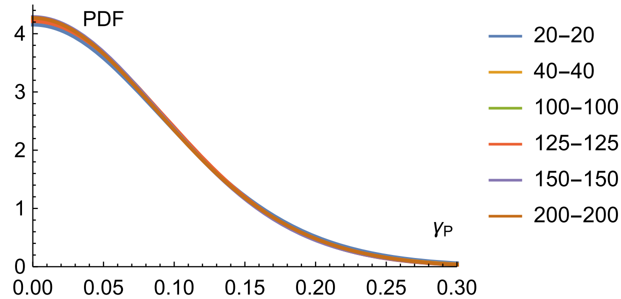

Fig. 2 The probability density functions of internal resistance γ_P for neutral equilibrium dislocation ensembles; number of dislocations in periodic cell is shown in the legend. Probability density functions are even, and only the dependence on positive γ_P is shown

In summary, periodic systems of edge dislocations seem to follow the similitude principle of cell structures (1) rather than the glide resistance strengthening associated with Taylor's relation (2). There are two alternative views on this proposition. First, it might be that 2D periodic dislocation structures differ considerably from 3D random structures. It is likely that an periodicity of the dislocation ensemble makes the unavoidable imprint on the overall behavior in two dimensions. Such an imprint can be due to the long-range character of 2D dislocation interactions. A "warning sign" has been seen already in the formula for the energy density of 2D periodic dislocation ensembles [8]: The energy density turns out to be dependent on the cell size no matter how complex the random content of the cell is. This is in contrest to other 2D periodic structures with random contents of the cell, like composites, where the results are independent of the cell size if the correlation radius is much smaller than the cell size. Usually, periodic structures are perceived as a model of random structures with cells being similar to representative volume elements. The very dependence of energy and characteristics like the yield strength on the cell size makes continuum theories of dislocations principally different from classical continuum models.

It is a possible alternative view that a considerable increase in the number of dislocations, well beyond 400 presented in Fig. 2, will bring the formation of a large number of small dislocation cells, which take the ultimate control of the yield stress. The yield strength becomes proportional to the inverse size of dislocation cells and, thus, to the square root of dislocation density in full agreement with Taylor's formula. Besides, the yield strength is independent of the cell size of the periodic structure. Though such a scenario is not impossible, it seems unlikely due to the very fast conversion of the probability density of the internal resistance shown in Fig. 2. This issue requires further analytical and numerical study.

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