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Abstract

We propose a mesoscopic model that explains the factor of two to three discrepancy between experimentally measured yield stresses of BCC metals at low temperatures and typical Peierls stresses determined by atomistic simulations of isolated screw dislocations. The model involves a Frank-Read type source emitting dislocations that become pure screws at a certain distance from the source and, owing to their high Peierls stress, control its operation. However, due to the mutual interaction between emitted dislocations the group consisting of both non-screw and screw dislocations can move at an applied stress that is about a factor of two to three lower than the stress needed for the glide of individual screw dislocations.

Keywords

Comments

Explanation of the discrepancy between the measured and atomistically calculated yield stresses in body-centered cubic metals

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Abstract

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Keywords: Peierls stress; screw dislocations; mixed dislocations; interactions; Frank-Read sources

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1 Introduction

It has been firmly established by many experimental and theoretical studies performed in the last forty years that the plastic behavior of body-centered-cubic (BCC) metals is controlled by $1/2\langle 111\rangle$ screw dislocations the cores of which are non-planar (for reviews see [1-7]). However, the only direct experimental observation that suggests such core spreading is the high-resolution electron microscopic (HREM) study of Sigle [8]. On the other hand it was concluded in a very recent HREM study of screw dislocations in Mo [9] that the experimental noise masks the true structure of the dislocation core. Hence, the primary source of our understanding of the dislocation core structure and related atomic-level aspects of the glide of $1/2\langle 111\rangle$ screw dislocations is computer simulation. Such calculations have been made using a broad variety of descriptions of interatomic forces, ranging from pair-potentials [10-12] to density functional theory (DFT) based calculations [13-15] and studies employing other quantum mechanics based methods [16-18].

The vast majority of atomistic studies of the core structure and glide of $1/2\langle 111\rangle$ screw dislocations in BCC metals were carried out using molecular statics techniques and thus they correspond to 0 K. A problem encountered universally in all the calculations of the critical resolved shear stress (CRSS), i.e. the Peierls stress, at which the screw dislocation starts to glide, is that it is by a factor of two to three larger than the CRSS obtained by extrapolating low-temperature experimental measurements of the yield and flow stresses to 0 K. The following are a few examples. Basinski et al. [19] measured the flow stress of potassium in the temperature range 1.5 K to 30 K and extrapolated to 0 K to get 0.002μ to 0.003μ where $\mu=(C_{11}-C_{12}+C_{44})/3$ is the $\langle 111\rangle\{110\}$ shear modulus and C_{11}, C_{12}, C_{44} are elastic constants. Similar values were found by Pichl and Krystian [20]. The values of the CRSS when the maximum resolved shear stress plane (MRSSP) is a $\{110\}$ plane, calculated using a pair potential derived on the basis of the

theory of weak pseudopotentials [21], is 0.007μ to 0.009μ [19]. More recently, Woodward and Rao [14] calculated the CRSS in molybdenum using the many-body potentials derived from the generalized pseudopotential theory [22] and a DFT based method. When the MRSSP is a {110} plane, they found the CRSS to be between 0.018μ and 0.020μ. A similar value of the CRSS, 0.019μ, was found in calculations employing the tight-binding based bond-order potential for molybdenum [18, 23]. Experimental measurements of Hollang et al. [24], extrapolated to 0 K, give for the CRSS in molybdenum 0.006μ. A similar problem was encountered by Wen and Ngan [25] who used the Embedded Atom Method (EAM) potential for iron and the Nudged Elastic Band method to analyze the activation enthalpies for kink-pair nucleation on screw dislocations. The calculated yield stress at 0 K was about 0.013μ.Similar values of the Peierls stress were found in recent calculations of Chaussidon et al. [26] who also employed EAM type potentials for iron. In contrast, the experimental values, reported by Aono et al. [27] are 0.005μ to 0.006μ. This ubiquitous higher value of the calculated CRSS, found independently of atomic interactions, suggests that the origin of this discrepancy cannot be sought on the atomic scale of the motion of individual dislocations but rather on mesoscopic scale where a large number of elastically interacting dislocations glide at the same time. In this context it should be noticed that the only atomistic simulation that predicts yield stress close to that measured experimentally considered a planar dislocation network of 1/2[111] and 1/2[$\bar{1}\bar{1}$1] screw dislocations with [001] screw junctions [28]. Such a network moved in the ($\bar{1}$10) plane at the stress about 50% lower than the Peierls stress of an isolated screw dislocation.

In-situ TEM observations of dislocation sources in BCC transition metals showed that in thin foils straight screw dislocations formed near the source and moved very slowly as a group [29-35]. Hence they fully control the rate at which the source produces dislocations. In the foils used in TEM the applied stresses are very low but a similar control of the sources by sessile screw dislocations can be expected in the bulk at stresses leading to the macroscopic yielding. However,

at higher stresses dislocations move faster and do not become pure screws immediately after leaving the source but at a distance from the source. Indeed, even in situ observations at higher stresses do not show straight screw dislocations emanating directly from the sources [36].

In this paper, we propose a mesoscopic model involving a Frank-Read type source [37] emitting dislocations of generally mixed character that become pure screw dislocations at a distance from the source and, owing to their high Peierls stress, control its operation. However, there are a number of non-screw dislocations between the screws and the source, which can move easily. These dislocations exert a stress on the screw dislocations and this stress, together with the applied stress, act on the screw dislocations by the force equal to that needed to overcome the Peierls stress. Screw dislocations can then move at an applied CRSS that is about a factor of two to three lower than the CRSS needed for the glide of individual screw dislocations.

2 Model of dislocation nucleation and motion

Let us consider a Frank-Read source (see e.g. [37]) that produces dislocations in a BCC metal. It emits, as always, dislocation loops that have a mixed character and expand easily away from the source since their Peierls stress is low. However, at a certain distance from the source, a significant part of the expanding loop attains the screw orientation and becomes much more difficult to move owing to the very high Peierls stress of pure screws. The rest of the loop, having a mixed character, continues to expand which leads to further extension of the screw segments. As a result, the source becomes surrounded by arrays of slowly moving screw dislocations, as depicted schematically in Figure 1. Further operation of the source is hindered by their back stress and effectively controlled by the ability of the screw dislocations to glide.

[Insert figure 1 about here]

The operation of the source is driven by the applied shear stress, σ_a, parallel to the slip direction, which acts by the Peach-Koehler force [37] $\sigma_a b$ (per unit length) on the dislocation that bows out. This dislocation obviously has a mixed character. Let us consider now that there are N_s screw dislocations at distances x_i from the source and N_m dislocations, generally of mixed character, positioned between the source and the screw dislocations. We approximate the latter as straight lines of the same orientation as the screws, positioned at distances y_k from the source, but with a negligible Peierls stress compared to that of the screws. In the framework of the isotropic elastic theory of dislocations the condition for the source to operate is then

$$\sigma_a b \geq \frac{\tau}{R} + \frac{\mu b^2}{2\pi\alpha} \sum_{i=1}^{N_s} \frac{1}{x_i} + \frac{\mu b^2}{2\pi\beta} \sum_{k=1}^{N_m} \frac{1}{y_k} \quad , \tag{1}$$

where τ is the line tension of the emitted dislocations, b their Burgers vector, R the half-length of the source, μ the shear modulus, and α, β constants of the order of unity. The first term is the force arising from the line tension that pulls the dislocation back and the second and third terms are forces produced by the stress fields of screw and non-screw dislocations, respectively, present ahead and/or behind the source. In the following we neglect the interaction between dislocations ahead and behind the source as they are far apart. Moreover, the dislocation sources are frequently single-ended (see e.g. [37]). Hence we analyze only dislocations ahead of the source, i.e. those towards which the source bows out.

It should be noted here that the screw dislocations in the array ahead of the source are not pressed against any obstacle and thus they do not form a pile-up. Within the approximations defined above, the ith screw dislocation will move provided

$$\sigma_a + \frac{\mu b}{2\pi}\sum_{\substack{j=1 \\ j\neq i}}^{N_s}\frac{1}{x_i - x_j} + \frac{\mu b}{2\pi\alpha}\sum_{k=1}^{N_m}\frac{1}{x_i - y_k} + \frac{\mu b}{2\pi\alpha}\frac{1}{x_i} \geq \sigma_P \quad , \tag{2}$$

where σ_P is the Peierls stress of screw dislocations. The second and third terms are stresses arising from screw and non-screw dislocations, respectively, and the fourth term is the stress arising from the dislocation associated with the source that is also treated as a straight line of the same type as all the other mixed dislocations. Since the Peierls stress of non-screw dislocations is negligible, the ℓ th non-screw dislocation can move provided

$$\sigma_a + \frac{\mu b}{2\pi\alpha}\sum_{j=1}^{N_s}\frac{1}{y_\ell - x_j} + \frac{\mu b}{2\pi\beta}\sum_{\substack{k=1 \\ k\neq\ell}}^{N_m}\frac{1}{y_\ell - y_k} + \frac{\mu b}{2\pi\beta}\frac{1}{y_\ell} \geq 0 \quad . \tag{3}$$

The meanings of individual terms are analogous to those in equation (2).

Now, the question asked is how large stress, σ_a, needs to be applied so that the screw dislocations can move so far away from the source that they either reach a surface or encounter dislocations of opposite sign from another source and annihilate, which leads to the propagation of slip through the sample. In both cases the source then keeps producing new dislocations indefinitely and the sample deforms plastically. In order to investigate the problem formulated above, we performed the following self-consistent simulations for certain fixed values of the Peierls stress, σ_P, and applied stress σ_a. First, we choose a half-length of the source, R, and a distance from the source, y_{max}, beyond which the expanding loop always attains the screw character. The first mixed dislocation emitted by the source becomes screw when reaching the distance y_{max} and then moves to a distance x_1, determined by equation (2). Provided that the source can operate, i.e. the inequality (1) is satisfied, another dislocation is emitted from the source. The position of this dislocation is determined by equation (3) if it does not reach y_{max} and

by equation (2) if it does. Subsequently, the position of the first dislocation, x_1, is updated to satisfy equation (2), which allows also the second dislocation to move. In this way a new position of the first dislocation, x_1, and the position of the second dislocation, either y_1 if smaller than y_{max} or x_2 if larger than y_{max}, are found self-consistently. This self-consistent process is then repeated for the third, fourth, etc., dislocations until the source cannot emit a new dislocation, i.e. when inequality (1) is no longer satisfied. The result of this calculation is the number of screw dislocations, N_s, and mixed dislocations, N_m, as well as their positions ahead of the source, when the source becomes blocked by the back-stress from all the emitted dislocations. The first screw dislocation is then at a position $x_1 = x_{max}$ and further operation of the source can proceed only if this screw dislocation is removed, as argued above. The source can then continue operating in a steady-state manner, producing a large number of dislocations that mediate the macroscopic plastic flow.

3 Results

In the following numerical simulations the applied stress, σ_a, has been set equal to $0.3\sigma_P$ and $0.5\sigma_P$, respectively, in order to investigate whether the source can operate at stress levels corresponding to experimental yield stresses extrapolated to 0 K, as discussed in the Introduction. Three values of the Peierls stress, σ_P, have been considered that fall into the range found in atomistic studies of transition metals [14, 18, 23, 25], namely 0.01μ, 0.02μ, and 0.03μ. Three different positions at which mixed dislocations transform into screw ones have been considered, namely $y_{max}/b = 500$, 1000, and 2000. The dependence on the size of the source, R, was also investigated. However, this dependence is very weak since R enters only through the line tension term in (1) and this is always small compared to the terms arising from the back-stress of emitted

dislocations. Hence, without the loss of generality, we set $R=y_{max}$. Moreover, the non-screw dislocations considered in the model deviate only slightly from the screw orientation and thus the difference between their long-range stress fields and those of screws is negligible compared to the orders of magnitude difference in their Peierls stresses. Hence, the values of parameters α and β in Eqs. (1) to (3) have been set to one. Finally, the usual approximation for the line tension, $\tau=\mu b^2/2$ [37], is adopted.

[Insert figure 2 about here]

Results of such simulation are presented in detail for $\sigma_a=0.5\sigma_P$, $\sigma_P=0.02\mu$ and $y_{max}=500b$ in Figure 2, where positions of the dislocations ahead of the source and stresses acting on them are shown. In this case $x_{max}/y_{max}=1.8$. It should be noted that the stress exerted on the majority of screw dislocations is practically equal to their Peierls stress. The distances x_{max} found for the two values of σ_a, three values of σ_P and three values of y_{max}, are summarized in Table 1.

[Insert table 1 about here]

These results suggest that, for a given applied stress, the ratio x_{max}/y_{max} is almost constant, independent of y_{max}, and only weakly dependent on the magnitude of the Peierls stress σ_P. At $\sigma_a/\sigma_P=0.3$, most of the dislocations are mixed and $x_{max}/y_{max}\approx1.3$. With increasing stress, more emitted dislocations become screw and, at $\sigma_a/\sigma_P=0.5$, $x_{max}/y_{max}\approx2$, which implies that the numbers of mixed and screw dislocations ahead of the source are very similar. Very importantly, the stress exerted on most of the screw dislocations is practically equal to their Peierls stress, see Figure 2.

4 Conclusion

The distinguishing characteristic of the model presented in this paper is that it does not consider the glide of a single screw dislocation but movement of a large group of dislocations produced by a Frank-Read type source. In general, this source produces dislocation loops of mixed character that transform into pure screws at a distance y_{max} from the source. Hence, the group of dislocations consists of screw dislocations at distances larger than y_{max} and non-screw dislocations near the source. It is then the combination of the applied stress with the stress produced by the dislocations in this group that acts on the screw dislocations and is practically equal to their Peierls stress. However, after emitting a certain number of dislocations the source becomes blocked by their back-stress and, at this point, the leading screw dislocation reaches the distance x_{max} from the source. Nonetheless, the source can continue operating if a dislocation of opposite sign, originating from another source, annihilates the leading screw dislocation (see Figure 3). This requires an average separation of sources about $2x_{max}$. Since the pinning points of the sources are produced by intersections with dislocations in other slip systems, their separation is related to the dislocation density in these systems. In a deformed molybdenum crystal this density is of the order of $10^{12}\,\mathrm{m}^{-2}$ [38] which implies separation of dislocations between $3000b$ and $4000b$, for the lattice parameter of Mo equal to 3.15 Å. These values are in the range of $2x_{max}$ for applied stresses that are between one-third and one-half of the atomistically calculated Peierls stress.

[Insert figure 3 about here]

The present study implies that the Peierls stress of screw dislocations in BCC metals found in atomistic studies cannot be compared directly with the measured yield stress extrapolated to 0 K.

The experiments do not determine the stress needed for the glide of individual screw dislocations but, instead, the stress needed for the operation of sources that are hindered by the sessile screw dislocations. These sources can operate at stresses lower than the Peierls stress of the screws owing to the collective motion of screw and mixed dislocations produced by them, as described in this paper. Hence, the discrepancy between the calculated Peierls stress and the measured yield stress is not a consequence of the inadequacy of the description of atomic interactions, which has often been raised as a possible explanation, but impropriety of their direct comparison.

Acknowledgments

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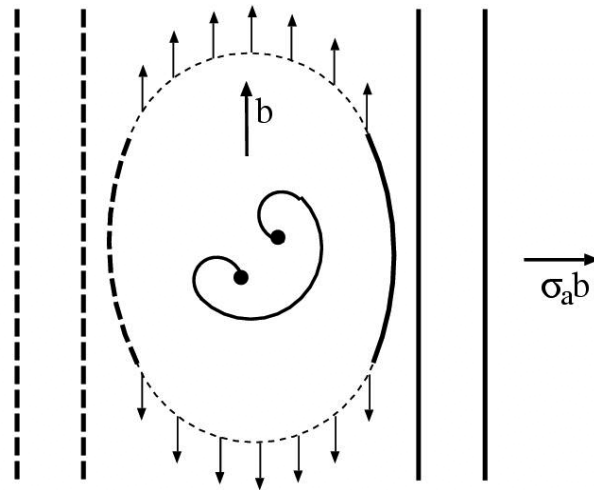
Figure 1: Schematic operation of a dislocation source in bcc metals. The curved non-screw segments migrate away, leaving behind a new pair of screw dislocations. σ_a is the shear stress in the slip plane acting parallel to the slip direction and $\sigma_a b$ the corresponding Peach-Koehler force exerted on dislocations produced by the source.
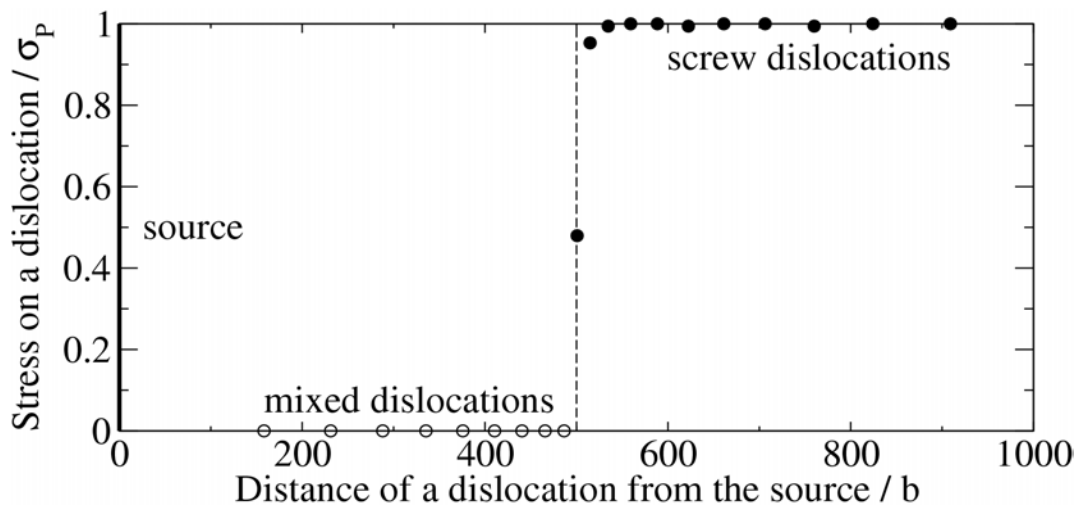
Figure 2: Positions of mixed (open circles) and screw (full circles) dislocations and the corresponding stresses when the source is blocked by the back-stress for the case $\sigma_d/\sigma_P{=}0.5$, $\sigma_P/\mu{=}0.02$, and $y_{max}/b{=}500$.

Table 1: The distance which the leading screw dislocation advances from the source, x_{max}, as a function of the distance y_{max} from the source at which dislocations become screw, for the applied stress σ_a/σ_P and the Peierls stress of the screw dislocations σ_P/μ.

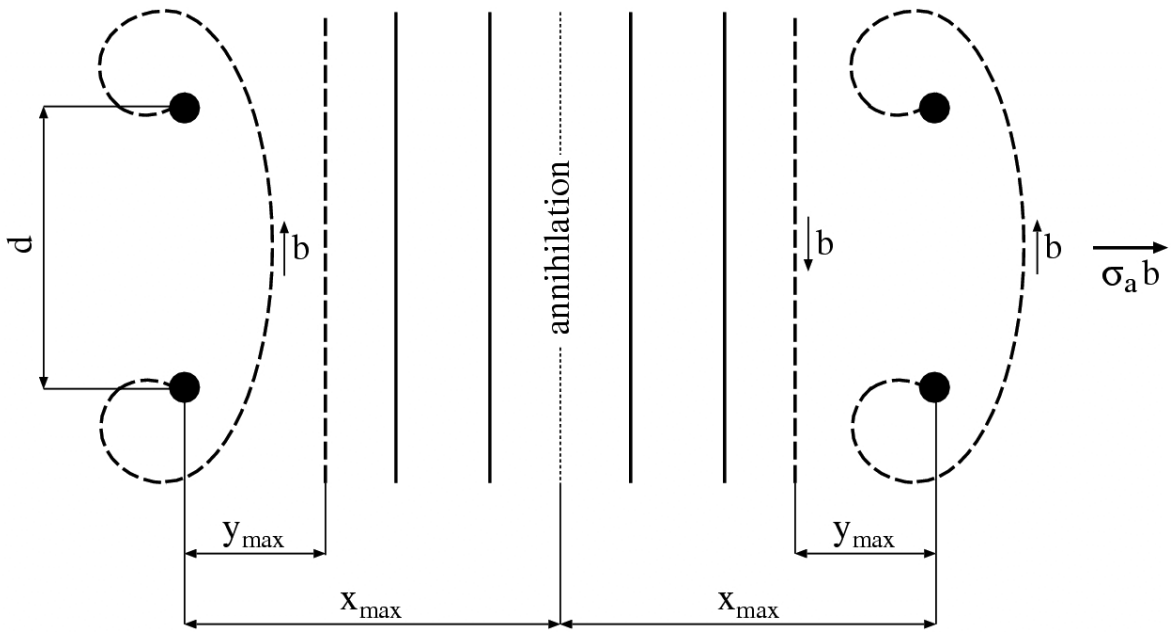|		y_{max}/b		
		500	1000	2000
	$\sigma_a/\sigma_P=0.3$			
	$\sigma_P/\mu=0.01$	1.0	1.1	1.2
x_{max}/y_{max}	$\sigma_P/\mu=0.02$	1.2	1.3	1.3
	$\sigma_P/\mu=0.03$	1.2	1.2	1.2
	$\sigma_a/\sigma_P=0.5$			
	$\sigma_P/\mu=0.01$	1.6	1.8	2.0
x_{max}/y_{max}	$\sigma_P/\mu=0.02$	1.8	2.0	2.0
	$\sigma_P/\mu=0.03$	1.9	2.0	2.0

Figure 3: When two dislocations of opposite Burgers vectors, generated by different sources, annihilate at a distance x_{max}, the reduced back-stress on the sources allows a steady-state generation of new dislocations. $\sigma_a b$ is the Peach-Koehler force exerted on dislocations by the applied shear stress σ_a.