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# An analysis of the pile-up of infinite periodic walls of edge dislocations

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ABSTRACT

We analyse the equilibrium pile-up configurations of infinite periodic walls of edge dislocations which are forced against an impenetrable obstacle by a constant applied shear stress. Numerically generated density distributions exhibit two distinct regions, for each of which we provide an interpretation and an analytical prediction. Near the obstacle, the influence of neighbouring slip planes may be neglected and the classical solution for a single slip plane applies. At a larger distance a linear decay is obtained. The characteristic length scales of the two parts of the pile-up are shown to depend differently on the parameters of the problem.



## 1. Introduction

Grain boundaries, second-phase particles and other heterogeneities in the microstructure of polycrystalline materials have a pronounced effect on the material's overall inelastic response. Their presence impedes the glide of dislocations and thus allows a smaller amount of local plastic deformation at a certain applied stress. Heterogeneities in the dislocation density which thus arise are the cause of so-called size effects, i.e. a dependence of the macroscopically measured mechanical response on the spatial scale (size) of the microstructure. A well-known example is the Hall–Petch effect (Hall, 1951; Petch, 1953) of the average grain size on the yield strength of a polycrystal.

These observations, among others, inspired researchers from the mid-20th century onwards to theoretically study the pile-up of dislocations against impenetrable obstacles (see e.g. Eshelby et al., 1951; Leibfried, 1951; Head and Louat, 1955; Chou and Whitmore, 1961; Chou, 1967; Pande, 1970). Due to the discrete nature of dislocations and the stress fields emitted by them, individual dislocations of the same sign (or orientation and Burgers vector) generally repel each other. This implies that, as some of them get stuck at an obstacle, those that follow remain at a finite distance from the first one and from each other. As a result, a boundary layer is formed along the obstacle, with an increased dislocation density, which however decays with increasing distance from the obstacle – a pile-up.

Many of the existing studies of pile-ups aim at characterising, or predicting, the dislocation density profile leading up to the obstacle. The earliest studies consider a linear array of edge or screw dislocations on a single glide plane. For this case, first studied in a discrete setting in the classical paper by Eshelby et al. (1951), Leibfried (1951) and Head and Louat (1955) established a continuous solution which essentially shows a $1/\sqrt{x}$ dependence of the dislocation density on the distance $x$ to the obstacle. Subsequent studies of the interaction between linear pile-ups on different glide planes, or in fact on a family of glide planes, have shown that such interactions may significantly influence the density profile (see e.g. Head and Louat, 1955; Chou and Whitmore, 1961; Louat, 1963; Chou, 1967; Pande, 1970). In particular, Louat (1963) established an analytical density distribution for an infinite stack of linear pile-ups of screw dislocations. This distribution differs significantly from the classical $1/\sqrt{x}$ decay and shows a dependence on the spacing of the glide planes on which the pile-ups live.

Roy et al. (2008) performed a numerical study of infinite walls of screw and edge dislocations. For this study, infinite dislocation walls piling-up against an obstacle perpendicular to their glide planes were selected because this particular configuration has short-range stresses only, and is thus ideally suited to examine their effect. For screw dislocations, the numerically computed dislocation density profiles corresponded well with the analytical solution by Louat (1963). For edge dislocations, no closed-form solution appeared to be available in the literature. In the numerical simulations, the classical $1/\sqrt{x}$ decay of the dislocation density was observed close to the obstacle, which at somewhat larger distances transitioned into another, unknown dependence.

More recently, Hall (2011) has established, by a rigorous discrete-to-continuum transition, that the density profile at some

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distance from the obstacle becomes linear. Numerical solutions of the discrete problem are shown to largely follow this linear dependence, apart from boundary layers at the head and tail of the pile-up. Hall also discusses the physical relevance of the assumption that the walls are periodic and concludes that walls are likely to emerge on non-periodic (active) slip planes as well, but the interactions between such non-periodic walls may be quite different from the periodic case.

Related studies of parallel pile-ups have been done by Baskaran et al. (2010) and Schouwenaars et al. (2010). In particular, Baskaran et al. (2010) studied a double-ended pile-up problem in which the slip planes are oriented at an arbitrary angle with respect to the obstacles. For angles other than 90°, long-range stress fields exist that are shown to be dominant in the formation of the pile-up. In the "degenerate" case of exactly 90° no such long-range stresses exist and the approach followed cannot be used. Schouwenaars et al. (2010) examined the influence of various idealisations – in particular of the assumption of infinite dislocation walls and infinite dislocation lines. They correctly argue that finite walls of dislocations have long-range stress fields and that these may overwhelm the short-range stresses emitted by the individual dislocations – see e.g. also Lubarda and Kouris (1996). Interestingly, they argue that regardless of this difference the equilibrium positions are similar for both configurations.

In this paper we return to the case of infinite walls of edge dislocations piling up against a parallel obstacle considered also by Roy et al. (2008) and by Hall (2011). We would like to emphasise that this case is highly idealised in many respects. Dislocation structures encountered in real materials obviously are unlikely to be perfectly periodic and neither are they infinite. But perhaps more importantly, in real materials multiple slip systems are available and additional mechanisms such as cross-slip and climb may become active. We nevertheless believe the idealised case of periodic single slip is worth studying more closely for three reasons: (i) it allows us to study the effect of short-range stresses in dislocation interaction in a clear, transparent setting, where it is not cluttered by other effects (see also Roy et al., 2008); (ii) in particular, it allows us to study the influence of mutual interaction between different glide planes, depending on their spacing; (iii) it emphasises once more the importance of accounting properly for the discreteness of dislocations and their interactions (Roy et al., 2008; Hall, 2011).

The purpose of this paper is threefold. Firstly, we confirm the linear density profile predicted by Hall (2011) via an alternative, more heuristic route. Secondly, we show that near the obstacle this profile transitions into the $1/\sqrt{x}$ dependence observed by Roy et al. (2008) and that this "boundary layer" (in the terminology of Hall, 2011) may thus also be described by a continuous density. And thirdly, we show that depending on the parameters of the problem, on of the two regimes may be dominant, or both occur at the same time. In the latter case, a fairly good prediction of the entire pile-up, including the transition point between the two regions, is obtained by combining the two analytical expressions.

The remainder of this paper is organised as follows. Section 2 defines the discrete dislocation pile-up problem which we study here and presents the numerical solutions which we use as a reference throughout the paper. The two regions which can be distinguished in the numerical data are analysed individually in Sections 3 and 4, whereas the transition between them is discussed in Section 5. We close with a brief summary of conclusions in Section 6.

## 2. Numerical solution of the discrete pile-up problem

We consider the problem of a pile-up of edge dislocations against an impenetrable obstacle, as sketched in Fig. 1. The dislocations, denoted by ⊥ in the figure, live on an infinite number of equally spaced slip planes at $y \in \{0, \pm h, \pm 2h, \ldots, \pm\infty\}$. The dislocations lines are all assumed to be straight and perpendicular to the $x$–$y$ plane. Their Burgers vectors, which are all of equal length $b$, are aligned with the positive $x$-axis. It is furthermore assumed that the dislocations are arranged in infinite vertical walls and that this wall structure is preserved at all times, i.e. the dislocations within a single wall only move collectively and uniformly. The horizontal positions of the walls are denoted $x_i$, where $i = 0, 1, 2, \ldots, n$. The first wall is immobilised at $x = x_0 = 0$ and acts as an obstacle for all other walls; $n$ thus denotes the number of mobile dislocation walls.

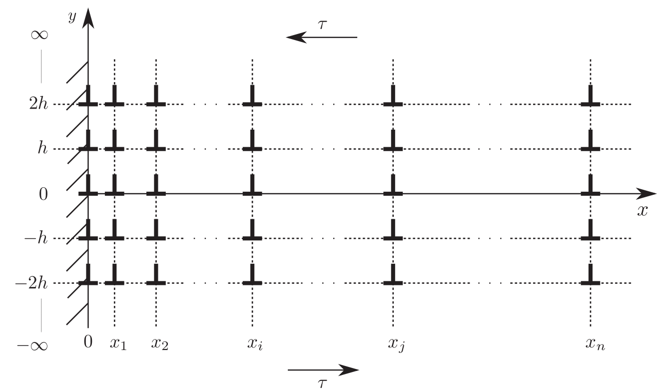


**Fig. 1.** Pile-up of vertical walls of edge dislocations in an infinite elastic medium. The dislocation wall at $x = 0$ is immobile.

The system of dislocation walls is embedded in an infinite linear elastic medium which is characterised by its shear modulus $G$ and Poisson's ratio $\nu$. It is subjected to a remote, constant shear stress $-\tau$. As a result of this applied stress and the interaction between the individual walls, the dislocation walls form a pile-up against the immobile wall at $x = 0$. We are interested in establishing the equilibrium pile-up configuration, i.e. the positions of the walls at rest.

The stress field emitted by a single dislocation wall can be obtained by summing up the classical expressions for a single dislocation due to Volterra for all dislocations within the wall (Hirth and Lothe, 1992). Since only the shear component contributes to the Peach–Koehler force experienced by another dislocation and since all glide planes within the infinite crystal considered are identical, we limit ourselves to the shear stress acting on the glide plane at $y = 0$. At the position of wall $i$, the stress due to the presence of wall $j$ equals:

$$\sigma_{xy} = \frac{\overline{G}b}{h} \frac{(\pi/h)(x_i - x_j)}{\sinh^2((\pi/h)(x_i - x_j))} \tag{1}$$

wherein the elastic constant $\overline{G}$ is defined as

$$\overline{G} = \frac{G}{2(1-\nu)} \tag{2}$$

A given wall $i$, where $1 \le i \le n$, reaches equilibrium when the stress fields due to all other walls cancel the externally applied stress, i.e. when

$$\sum_{\substack{j=0 \\ j \neq i}}^{n} \frac{(\pi/h)(x_i - x_j)}{\sinh^2((\pi/h)(x_i - x_j))} = \frac{\tau h}{\overline{G}b} \tag{3}$$

For the immobile wall at $x = 0$ to be in equilibrium, a reaction stress equal to $(n+1)\tau$ must be added to this equation (Eshelby et al., 1951). However, since the position of this wall is already known, the resulting equation can be disregarded in what follows.