Multiple dislocation pile-ups in small grains at small strains: implications for the Hall-Petch relationship and backstress screening

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Abstract. A classic explanation for the Hall-Petch relationship is given by the stress field of a single dislocation pile-up perpendicular to the grain boundary. Similarly, the gradual compensation of the stress fields of pile-ups on both sides of the boundary has been invoked to explain the transitory effects observed in the stress-strain curves of ultrafine grained polycrystals. This paper studies the effects of introducing deviations of the highly simplified geometry mentioned above, using the proper mathematical approximations of linear elastic dislocation theory. Multiple pile-ups invalidate the conclusions drawn from the single pile-up model. Pile-ups in multiple grains are assessed by a highly idealised model of an infinite array of periodical pile-ups. In the latter case, screening is always perfect. By considering the Peach-Köhler force between dislocations mutually disoriented grains, the magnitude of the fluctuations around such ideal case can be estimated. However, using sound probabilistic arguments to calculate the free path for dislocation slip in fine-grained polycrystals, it is found that the amount of dislocations that can be stored in the pile-ups is generally too small to explain the strong grain size effects observed experimentally.

1. Introduction

The increase of the strength of metal polycrystals with decreasing grain size is commonly referred to as the Hall-Petch effect due to the two authors [1,2] who described their observations as:

\[ \sigma_y = \sigma_\infty + k d_g^{-1/2} \]  

(1)

where Hall studied the yield strength \( \sigma_y \) and Petch the brittle fracture stress of steels. \( \sigma_\infty \) is the yield stress of an infinite medium without grain boundaries, \( k \) an empirical constant and \( d_g \) the grain diameter. The relationship to dislocation pile-ups at grain boundaries is readily made by the classical analysis of a double pile-up in a single crystal embedded in an infinite elastic medium [3]. For the configuration presented in fig. 1a, one finds the following basic results:

\[ N = \frac{\pi(1-\nu)\sigma}{\mu b} d_g \]  

(2)
with \( N \) the total number of dislocation dipoles in the double pile-up, \( \nu \) Poisson’s coefficient, \( \mu \) the shear modulus and \( \sigma \) the resolved shear stress of the slip system considered. Assuming that there is a critical value of the Peach-Köhler (PK) force \( F_{PK} \) (expressed per unit length of dislocation) at which plastic strain is transmitted to the neighbouring grain, one finds:

\[
\sigma_y = \sqrt{\frac{4\mu}{\pi(1-\nu)}} F_{PK} d_g^{-1/2}
\]

(3) Provides a theoretical basis for (1). Plastic strain transmission may occur by the bow-out of a dislocation segment from the first grain to the second [4-7] or by the activation of dislocation sources in the neighbouring grain [5-8]. Numerical simulations provide estimates in the range of 1 to 2 GPa for these phenomena to occur in selected high-angle grain boundaries in Ni [9] and of 0.4 to 1 GPa for different low-angle grain boundaries in \( \alpha \)-iron [10,11].

In a more recent application, the concept of parallel pile-ups has been used to explain the stress maximum at low strains in the tensile curves of fine-grained materials [12,13]. It is considered that the gradual build-up of dislocation pile-ups on both sides of the grain boundary leads to a “screening” of the backstress fields of the same, i.e. the stress first builds up and then decreases to give way to a normal strain hardening behaviour as predicted by the Kocks-Mecking model [14]. The concept of screening has been developed in the context of the electron gas (see e.g. [15]). While the analogy between an electric line charge and a dislocation in an infinite elastic medium is easy to establish [16], other equations based on the statistical thermodynamics of the electron gas (e.g. the Thomas-Fermi equation) do not have any meaning in the description of dislocation distributions. Results from the statistical theory of the electron gas can therefore not be applied indiscriminately to the study of dislocation distributions.

The double pile-up, perpendicular to the boundary in a single grain, is evidently a huge simplification of what can be expected in real polycrystals. Multiple pile-ups can be expected and both the number of pile-ups and the number of dislocations in each pile-up are likely to be stochastic variables. In the latter case, any relationship to the Hall-Petch formula is lost. Chou and Li presented an extensive review of analytical solutions for discrete, distributed and multiple pile-ups [17], while Peerlings and co-workers have studied the behaviour of infinite arrays of pile-ups [18,19], i.e. the pile-ups of infinite low-angle grain boundaries against a high-angle boundary. Their results differ significantly from the more realistic configuration of a finite number of parallel pile-ups, which were studied by Schouwenaars et al. [20]. In the latter case, a significant long-range stress is found, which is nonetheless much lower than what is found if all dislocations are placed in a single pile-up (Fig. 1). Baskaran et al. studied the effect of the inclination of the pile-ups with respect to the grain boundary. They concluded that the perpendicular case is “pathological”, in the sense that it is a singular solution which is not representative for other angles [21].

![Fig.1. Comparison between the stress fields of 144 dislocations randomly distributed over 12 pile-ups compared to 144 dislocations in a single pile-up in a 1 \( \mu m \) grain (see ref. [20] for details).](image-url)
2. Infinite array of pile-ups

2.1. The model

Interactions between pile-ups in neighbouring grains have received relatively little attention. Nonetheless, they are essential if the concept of screening is to be understood more clearly. Therefore, an analytic model will be developed for an infinite array of identical grains in which pile-ups of opposite sign are present at both sides of each grain boundaries in a single slip plane. The degree of simplification is comparable to what is assumed when studying the double pile-up model for the single grain; as will be seen, both cases are limiting simplifications of what can be expected in real materials.

Fig. 2.b shows a periodic array of identical edge dislocations in the plane defined by their Burgers vector and line direction. An analytic solution for the stress field of this configuration is available [3]:

\[
\sigma_{xy} = \frac{\mu b}{2d_g(1-v)} \sin \left( \frac{2\pi x}{d_g} \right) \left( \cosh \left( \frac{2\pi y}{d_g} \right) \sinh \left( \frac{2\pi y}{d_g} \right) \cos \left( \frac{2\pi x}{d_g} \right) \right) \left( \cosh \left( \frac{2\pi x}{d_g} \right) + \cos \left( \frac{2\pi x}{d_g} \right) \right)
\]  

(4)

where it shall be noted that the reference frame is rotated 90° with respect to the original publication [3]. For y=0, i.e. in the slip plane, this simplifies to:

\[
\sigma_{xy} = \frac{\mu b}{2d_g(1-v)} \cot \left( \frac{\pi x}{\lambda} \right)
\]

(5)

Fig. 2.c shows how this configuration can be used to define an infinite array of dislocation dipoles. Using (5) it follows that the shear stress distribution is:

\[
\sigma_{xy} = \frac{\mu b}{2d_g(1-v)} \left( \cot \left( \frac{\pi(x-\delta)}{d_g} \right) - \cot \left( \frac{\pi(x+\delta)}{d_g} \right) \right)
\]

(6)

Fig. 2. a. Double pile-up in a single grain, with the continuous dislocation distribution and discrete dislocation positions marked. b. Single infinite array of dislocations equally spaced along the X-axis (formula 4). c. Array of pile-ups, with opposite dislocations separated by a distance \( \delta \) (formula 6). d. result of the calculations, with the continuous dislocation distribution along the grain diameter (formula 13). e. Simplified scheme to calculate the relationship between shear strain and number of dislocations on the slip system under consideration.

Assuming that the dislocations in the pile-ups are distributed according to a continuous function \( n(\delta) \), the stress equilibrium under an applied resolved shear stress \( \sigma \) is given by:
This is a singular integral equation which can be solved by the following series of substitutions:

\[ \cos \left( \frac{\pi \delta}{d_g} \right) = t \]

yielding:

\[ \sigma = \frac{\mu b}{2\pi(1-\nu)} \int_1^0 \frac{t}{t^2-u^2} n \left( \frac{d_g}{\pi} \arccos t \right) dt \]  

Next, substitute:

\[ t^2 = v \]
\[ u^2 = w \]

\[ n \left( \frac{d_g}{\pi} \arccos \sqrt{v} \right) = g(v) \]

yielding:

\[ \sigma = -c \int_0^1 g(v) dv \]

The latter equation is of a known form [21] and has the solution:

\[ g(v) = \frac{\sigma}{\pi^2 c} \sqrt{\frac{w}{1-w}} \int_0^1 \sqrt{\frac{1-z}{z-w}} dz \]  

which provides, after integrating and backsubstitution:

\[ n(\delta) = -4 \frac{\sigma(1-\nu) \cot \left( \frac{\pi \delta}{d_g} \right)}{\mu b} \]  

This result was obtained in a different way by Leibfried in 1951 [16] who did not further analyse its physical meaning; it was deemed useful to present the derivation here as a base for the analysis of its significance in terms of the grain size effect which follows.

2.2. Interpretation.

The number of dislocations in the pile-up at a given stress is determined by:

\[ N = 4 \frac{\sigma(1-\nu)}{\mu b} \int_0^{d_g/2} \cot \left( \frac{\pi x}{d_g} \right) dx \]

where ε is a cut-off radius which was taken equal to 1.5 \( b \). This radius would be equal to the zone where the dislocation could be considered to be part of the grain boundary rather than belonging to the pile-up. The value of this radius, in the context of the stress field of such grain-boundary dislocations, was discussed in detail by Vattré and Demkowicz [23].

It also follows that:

\[ n(x) = \frac{\pi \cot \left( \frac{\pi x}{d_g} \right)}{d_g \ln \left( \sin \left( \frac{\pi x}{d_g} \right) \right)} N \]

The equivalent super-dipole is defined as a pair of opposite dislocations on both sides of the GB, with Burgers vector equal to \( Nb \) and which produce the same long-range stress field as the \( N \) dislocations in the pile-ups. The separation of this dipole is found as:

\[ \delta_{eq} = -4 \frac{\sigma(1-\nu)}{N \mu b} \int_0^{d_g/2} x \cot \left( \frac{\pi x}{d_g} \right) dx \]  

or

\[ \delta_{eq} = \frac{d_g}{-2 \ln \left( \sin \left( \frac{\pi x}{d_g} \right) \right)} \]

This results in \( \delta_{eq} \approx 0.04d_g \), i.e. the pile-ups are concentrated within approximately
It is however not the stress field in the individual grain that determines the interaction. Multislip can be established as the superposition of the stress fields of the dislocations on the different slip systems in the polycrystal.

2.3. Stress-strain relationship.
An important result which follows immediately from (7) is that the internal stress in the polycrystal is now everywhere equal to the applied shear stress, i.e. screening is always perfect. Nonetheless, a stress-strain relationship can be obtained, using the geometry presented in fig. 2.e: shear strain is given by \( \varepsilon = \frac{b(1 - \delta_{eq})}{d_g} \frac{dN}{d} \)

Integrating and substituting for \( N \) and \( d_{eq} \), one finds:
\[
\sigma = \frac{\mu \gamma}{8(1-\nu)\left[\ln\left(\frac{d}{d_{eq}}\right) + \frac{d_{eq}\ln 2}{2}\right]}
\] (20)

For a given shear strain, one can then plot the yield stress against the grain size. Considering the conventional value of 0.2% tensile strain, which, for a Taylor factor of 3 corresponds to \( \gamma = 0.006 \), one finds the results given in fig. 3, in the form of a Hall-Petch plot (data for Cu). In the range where the HP-relationship is supposed to be valid, the plot is nonlinear and, for the idealised case developed here, the effect of the pile-ups is too small to explain the experimentally observed grain size effect.

![Fig. 3. Hall-Petch plot according to formula 20. Notice that the plot is non-linear in the range where the Hall-Petch relationship is usually considered valid and that the predicted grain size effect is small in comparison to what is generally reported.](image)

3. Stress fluctuations in the polycrystal.
3.1. Statement of the problem
Comparing the analysis of the infinite array of pile-ups to the classical analysis of a double pile-up in a single crystal, it follows that both are extreme cases of a simplified analysis in which all dislocations and slip systems are parallel. In the former, the backstress is always zero. In the latter, the backstress is completely unshielded by neighbouring pile-ups of opposite sign. The real situation can be expected to lie somewhere in between, consisting of a constant background with fluctuations which vary from grain to grain.

The reasons of these fluctuations are the different grain orientations in the polycrystal. At the early onset of deformation, favourably oriented grains will yield first, probably on a single slip system. However, the grain size effect is observed well beyond this initial stage [24] and at low values of tensile strain (e.g. 2%), multiple slip is already well-established [14, 25]. The long-range stresses of the local distribution of dislocations on the different slip systems in multislip can be established as the superposition of the stress fields of the dislocations on the individual systems, while the active slip systems can be determined by a suitable polycrystal plasticity code [26, 27].

It is however not the stress field in the individual grain that determines the interaction between dislocations in neighbouring grains, but the PK-force of the dislocations on a given slip system in one grain, working on the dislocations of another slip system in the
neighbouring one. This represents a topic of considerable complexity which is briefly explored in the following.

3.2. Analytic framework

The geometry studied is as follows: the boundary between grains 1 (to the left) and 2 (to the right) is taken to be the X_2-X_3 plane and the boundary is a square with sides equal to 1 centred on the X_1-axis. The slip systems are characterised by their unit normal vector \( \mathbf{n} \) and the unit slip vector \( \mathbf{b} \). The components of \( \mathbf{n} \) and \( \mathbf{b} \) are known in the crystal reference system of both grains. Let \( \mathbf{g}^\beta \) be the matrix of direction cosines of the crystal reference system \( \beta \) in the external reference system. To avoid any confusion and simplify the notation, the inverse of \( \mathbf{g}^\beta \) will be denoted \( \mathbf{h}^\beta = \mathbf{g}^\beta \).

All the following calculations are made in the external reference frame. The slip plane for system \( n^\alpha \) in crystal \( \beta \) through the origin is given by (summation only over Latin subscripts):

\[
h^\beta_{ij} n^{\alpha j} x_i = 0
\]  

(21)

The Burgers vector is given by

\[
b^\beta_{ij} = h^\beta_{ij} n^\alpha
\]  

(22)

The unit vector of the intersection of this plane with the crystal boundary is then given by:

\[
\xi^{\alpha j} \pm \frac{1}{\sqrt{(n_{2j} n_{2j}^\alpha)^2 + (n_{3j} n_{3j}^\alpha)^2}} \begin{pmatrix} 0, -h^\beta_{2j} n^{\alpha j}, h^\beta_{3j} n^{\alpha j} \end{pmatrix}
\]  

(23)

where the colon reads as: “has the components”. The sign of this vector has to be determined by the observation that the dislocation must move toward the GB under the applied stress \( \sigma \). Only the segment of the dislocations stored parallel to the GB will be considered. These segments can be stored at random locations along the boundary, as was studied in an earlier publication [20]. An average effect will be calculated for the dislocations spread homogeneously in a plane parallel with the (square-shaped) GB. Local fluctuations of the stress field are thereby overlooked but the long range interaction is the same.

The interaction energy between two dislocation segments of length \( l \) on slip system \( n^\alpha \) in grain 1 (left) and \( \alpha \) in grain 2 (right), is given by [3]:

\[
W_{12} = -\frac{\mu}{2\pi} \int_{-l/2}^{l/2} \int_{-l/2}^{l/2} \frac{1}{l} \left( [\mathbf{b}_{\alpha 1} \times \mathbf{b}_{\alpha 2}] \cdot (\mathbf{\xi}_{\alpha 1} \times \mathbf{\xi}_{\alpha 2}) \right) d\alpha_{11} d\alpha_{22}
\]  

(24)

\[
+ \frac{\mu}{4\pi} \int_{-l/2}^{l/2} \int_{-l/2}^{l/2} \left( [\mathbf{b}_{\alpha 1} \times \mathbf{\xi}_{\alpha 1}^1] \cdot (\mathbf{b}_{\alpha 2} \times \mathbf{\xi}_{\alpha 2}^2) \right) d\alpha_{11} d\alpha_{22}
\]  

With

\[
T_{ij} = \frac{\partial^2}{\partial x_i \partial x_j} ||\mathbf{p}_{\alpha 1} - \mathbf{p}_{\alpha 2}||
\]  

(25)

Now, because the dislocations are straight, the Burgers vectors and line direction vectors are constants. This means that all \( \mathbf{b} \) and \( \mathbf{\xi} \) can be written outside the integral sign. Also, the averaging procedure of the individual dislocations over the grain boundary implies that the integral can be executed over the square domain instead of along the individual dislocation lines. The Peach-Köhler force is then found by deriving expression (24) under the integral signs with respect to \( x_i \):

\[
F_1 = \frac{\partial W_{12}}{\partial x_1} = -\frac{\mu}{2\pi} \left( [\mathbf{b}_{\alpha 1} \times \mathbf{b}_{\alpha 2}] \cdot (\mathbf{\xi}_{\alpha 1} \times \mathbf{\xi}_{\alpha 2}) \right) I_0(\Delta x_1)
\]  

(26)

\[
+ \frac{\mu}{4\pi} \left( [\mathbf{b}_{\alpha 1} \cdot \mathbf{\xi}_{\alpha 1}^1] \cdot (\mathbf{b}_{\alpha 2} \cdot \mathbf{\xi}_{\alpha 2}^2) \right) I_0(\Delta x_1)
\]  

\[
+ \frac{\mu}{4\pi(1-v)} \left( [\mathbf{b}_{\alpha 1} \cdot \mathbf{\xi}_{\alpha 1}^1] \cdot I_{ij}(\Delta x_1) \cdot (\mathbf{b}_{\alpha 2} \times \mathbf{\xi}_{\alpha 2}^2) \right)
\]  

With:
\[ I_0(\Delta x_1, x_2^2, x_3^2) = \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \frac{\partial}{\partial x_1} dx_2^1 dx_3^1 \] (27)

and

\[ I_{ij}(\Delta x_1, x_2^2, x_3^2) = \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \frac{\partial T_{ij}}{\partial x_1} dx_2^1 dx_3^1 \] (28)

where the simple superscripts now refer to the rectangular coordinates in the vertical plane in grain 1 and 2 respectively, instead of a particular dislocation line and \( \Delta x_1 = x_1^2 - x_1^1 \). In spite of the simplifications, the analytic expressions of (27) and (28) are too complex to be handled routinely. Moreover, after integrating over the dislocations in grain 1, a second integration over the vertical square must be made in grain 2, to obtain the average force on the randomly distributed dislocations in grain 2. Numerical integration is thus unavoidable; the average influence of the dislocations in grain 1 on the ones in grain 2 is obtained as:

\[ J_0(\Delta x) = \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} I_0(\Delta x, x_2^2 dx_3^2) dx_2^2 dx_3^2 \] (29)

\[ J_{ij}(\Delta x) = \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} I_{ij}(\Delta x, x_2^2 dx_3^2) dx_2^2 dx_3^2 \] (30)

Some of the results are summarized in Fig. 4.

Fig. 4. a. \( I_0(\Delta x, x_2^2, x_3^2) \) calculated at a distance of 0.02 \( d_g \) at both sides of the GB. b. Values of the quadruple integrals as a function of the separation between the vertical planes. Off-diagonal elements integrate to zero in the calculations of the \( J_{ij} \). c. Graphical representation of the tensor components \( I_{ij}(\Delta x, x_2^2, x_3^2) \) calculated for dislocation interaction at a distance of 0.02 \( d_g \) at both sides of the GB.
3.3. Examples for given misorientations.
Each grain boundary is characterised by 5 parameters: three for the misorientation and two for the GB-plane normal. Each of the 12 slip systems in grain 1 can interact with the 12 systems in grain 2, although the total number of cases will be reduced by symmetry. A general treatment of the effect of grain interaction must therefore be made through a statistical analysis or can be limited to specific configurations analysed by polycrystal plasticity. Neither study has been undertaken at the time of writing. Two specific cases can be found: for parallel screws, when both crystals shear a $<100\rangle\{001\}$ orientation and parallel edges, for $<110\rangle\{111\}$ oriented grains (there would however be no grain boundary between identically oriented grains). The results for these cases are:

$$F_1 = \frac{\mu}{8\pi(1-\nu)}(J_{11}(x) + J_{22}(x)) \quad \text{(edge)}$$  \hspace{1cm} (31)

$$F_2 = \frac{\mu}{4\pi}J_0(x) \quad \text{(screw)}$$  \hspace{1cm} (32)

The strongest interactions are found if one of the grains has a $<110\rangle\{111\}$ orientation and the other takes specific misorientations with respect to the former. The maximum positive interaction is found for a dislocation with $n:1/\sqrt{3}\ (111) ; b:1/\sqrt{2}\ [110]$ in a $[1\overline{1}0](111)$ grain and the $n:1/\sqrt{3}\ (\overline{1}1\overline{1}) ; b:1/\sqrt{2}\ [011]$ dislocation in the neighboring grain (Fig. 5). The same slip system shows the minimum negative interaction with the $n:1/\sqrt{3}\ (1\overline{1}1) ; b:1/\sqrt{2}\ [110]$ slip system, at a different misorientation (Fig. 6). Notice that the sign of the interaction is irrelevant for the physics of the problem, because the sign of the dislocation line vector will always be such that the dislocation is pushed toward the GB and therefore, the interaction between dislocations on either side is expected to be attractive. This factor is not explicitly accounted for in the formulas presented here (it suffices to take absolute values).

![Diagram](image_url)

**Fig. 5.** Presentation of the $x_i$ component of the PK-force as a function of misorientation with the $n:1/\sqrt{3}\ (111) ; b:1/\sqrt{2}\ [1\overline{1}0]$ in a $[1\overline{1}0](111)$ grain and a $n:1/\sqrt{3}\ (\overline{1}1\overline{1}) ; b:1/\sqrt{2}\ [011]$ dislocation in a grain whose orientation is characterised by the Euler angles $(\phi, \Phi, \phi_2)$ (plots at $5^\circ$ intervals in $\phi$). White zones indicate low values of the interaction.
The evident fact that the dislocations in a pile-up must reach their position by crystallographic slip from a source seems to be tacitly omitted in many studies of plastic size effects. Rigorous statistical analysis \cite{28} confirms the intuitive result that, at low dislocation densities, the free path for dislocation travel becomes equal to one half of the grain diameter. With \( \gamma = b(\lambda)\rho \) and considering that \( \rho = 2n/d_g^2 \), with \( n \) the number of dipoles (\( n \) is also the number of dislocations piled up against a single GB on one side), one finds that \( \gamma \approx bn/d_g \).

For a given tensile strain, the value of \( \gamma \) is found by multiplying with the Taylor factor (\( M \approx 3 \)). Then, the number of dislocations at the grain boundary can be estimated as shown in table 1 for \( \varepsilon = 2 \times 10^{-3} \) for different grain diameters and using data for copper.

Table 1. Estimated number of dislocations required to reach a given tensile strain for different grain diameters and the corresponding stresses for the dipole in the infinite array of dipoles or the single crystal if the dislocations were concentrated in a single pile-up. The last column gives the "spearhead" stress at the tip of the double pile-up in the single grain.

| \( d_g \) (m) | \( N \) | \( \sigma \) (infinite) | \( \sigma \) (single) | \( \sigma \) (tip) |
|--------------|--------|----------------|----------------|-------------|
| \( 10^{-5} \) | 234    | 38 MPa         | 139 MPa        | 32.5 GPa    |
| \( 10^{-6} \) | 23     | 51 MPa         | 139 MPa        | 3.25 GPa    |
| \( 10^{-7} \) | 2.3    | 78 MPa         | 139 MPa        | 0.33 GPa    |
5. Discussion and Conclusions

The first part of this paper compares two pile-up models in which an idealised single slip system is considered. In the classical one, only one grain deforms plastically, while in the new one, all grains deform simultaneously. In the former case, the stress concentration of the pile-up is fully unshielded. In the second one, the stress field is everywhere equal to the externally imposed shear stress and shielding is complete. Both models are clearly the extreme cases of a single simplified approximation in which the local crystallography of the polycrystal is neglected. Such approximations have been quite common in the classical literature on dislocations [29,30]. The results obtained in this paper show that such simplification neglects many of the essential aspects of dislocation interaction in polycrystals. Coupling between the dislocations in neighbouring grains is not directly introduced by the stress field but trough the Peach-Köhler force which is disorientation dependent and therefore fluctuates over distances equal to the grain diameter. A strong PK-force between active slip systems in neighbouring grains will attract the pile-ups toward the GB, producing shielding of their stress field in both grains. Screening, in the sense of a complete neutralisation of long-range stresses, will never occur. A low PK-force means that the dislocations in both grains act independently, i.e. they do not shield each other nor promote activity on the slip systems in the neighbour.

Evidently, there will always be an interaction between some of the 144 possible combinations of slip systems, but if the systems are non-active, the number of dislocations involved will be low. Also, the interactions mapped in Fig. 5 and 6 are the strongest ones found in the entire misorientation space. In general, the difference between maximum and minimum force is lower than what is shown here and the “white zone” in the maps, i.e. the zone where interactions are low, is more extensive. Interactions between second-nearest neighbours, as follows from fig. 3.b, are small.

Weak interactions could be interpreted as supporting the original model of a double pile-up in a single grain which is not affected by the configuration of its neighbours. Even if this were the case, at a given magnitude of slip, the number of dislocations required to produce this slip is proportional to the grain size. Already in the range of 100 nm, the pile-up concept breaks down because only two dislocations are needed to reach the 0.2% tensile strain. This is well before the often-cited breakdown of the model due to the discrete nature of the dislocations in the pile-up [31], which is reached around 20 nm. The stress required to introduce these dislocations into the pile-up is actually independent of \( d \), i.e. the model most often used to explain the Hall-Petch relationship predicts that the 0.2% proof stress is independent of grain size. The so-called “spearhead stress”, which is supposed to mobilise dislocations in the neighbouring grain is equal to the applied stress times the number of dislocations. Somewhere between 100 nm and 1 \( \mu \)m, this stress would fail to reach the values mentioned in the introduction.

It is therefore concluded that, in spite of their almost universal acceptance, simple pile-up models cannot explain the grain size effect in a way which is consistent with the nature of polycrystalline plasticity. More detailed models, taking into account the complex disorientation-dependent nature of the interaction of dislocations between grains are needed to estimate the magnitude of the associated microstress fields. For small grains at small strains, and taking into account the existence of multiple pile-ups on multiple slip systems, the number dislocations involved may be so low that the stress fields become insignificant. Alternative explanations, such as rapid strain hardening due to the short path length or an increase of dislocation density close to the grain boundary must therefore be investigated into more detail.

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