We address the problem of an elastic wave coherently propagating through a two-dimensional polycrystal. The main source of scattering is taken to be the interaction with grain boundaries that are in turn modelled as line distribution of dislocations—a good approximation for low angle grain boundaries. First, the scattering due to a single linear array is worked out in detail in a Born approximation, both for longitudinal and transverse polarization and allowing for mode conversion. Next, the polycrystal is modelled as a continuum medium filled with such lines that are in turn assumed to be randomly distributed. The properties of the coherent wave are worked out in a multiple scattering formalism, with the calculation of a mass operator, the main technical ingredient. Expansion of this operator to second-order in perturbation theory gives expressions for the index of refraction and attenuation length. This work is motivated by two sources of recent experiments: firstly, the experiments of Zhang et al. (Zhang, G., Simpson Jr, W. A., Vitek, J. M., Barnard, D. J., Tweed, L. J. & Foley J. 2004 J. Acoust. Soc. Am. 116, 109–116.) suggesting that current understanding of wave propagation in polycrystalline material fails to interpret experimental results; secondly, the experiments of Zolotoyabko & Shilo who show that dislocations are potentially strong scatterers for elastic wave.

Keywords: dislocations; grain boundary; polycrystal; scattering function; multiple scattering; effective medium
1. Introduction

The propagation of sound in polycrystals has long been an object of study (for a review, see for instance Thompson 2002). Individual grains within a polycrystal are single crystals, each with its own orientation, separated by grain boundaries. While the material within each grain is the same, the orientation of the crystal axes is different and it is this contrast in anisotropy that is at the root of the way elastic waves will behave in a polycrystal. Following the pioneer works of Lifshitz & Parkhomovskii (1950), the general approach to study sound propagation in polycrystals has been to consider a theory in which the elastic constants of the grains fluctuate. Methods include multiple scattering (Stanke & Kino 1984), use of a second-order Born approximation on an individual scatterer (Hirsekorn 1982) and geometrical acoustics (Rokhlin et al. 1991). Recent experiments of wave propagation in single phase polycrystalline material (Zhang et al. 2004), however, appear to be quite at variance with current theoretical modelling, thus suggesting a need to revisit the issue of sound elastic wave propagation in polycrystals. At the same time, other experiments (Zolotoyabko et al. 2001; Shilo & Zolotoyabko 2002, 2003) have illustrated that wave scattering by dislocations can be significant.

Low angle grain boundaries are well described as arrays of aligned edge dislocations (see figure 1). This is why we propose in this paper to address the problem of wave scattering by dislocation segments, a problem that has been disregarded before. To clearly isolate this effect, we do not include in our analysis the scattering coming from the different elastic properties between grains. We only consider the grain boundaries as interfaces able to be the sources of the scattering, while the medium they limit is taken to be the same, namely homogeneous and isotropic.

The interaction between an elastic wave and a dislocation has been first analysed by Eshelby (1949, 1953) and Nabarro (1951) by use of an electromagnetic analogy. A different approach has been largely developed by Granato & Lücke (Granato & Lücke 1956a,b, 1966, 1981; Lücke & Granato 1981) who model the dislocation as a string driven by a scalar time-dependent stress. Eshelby & Nabarro noted that the waves are scattered by a dislocation, because their motion induced by the incoming wave generates the emission of a scattered wave. Thus, a description of this mechanism involves two steps: the knowledge of the law of motion of a dislocation in the presence of an incident wave, and a representation for the elastic field generated by the moving dislocation. As an integral representation for the velocity field generated by a moving dislocation was derived from the Navier equations by Mura in 1963, the general framework to obtain the equations for the motion of a dislocation in the presence of an incident wave is much more recent (Lund 1988). This is probably why little about the interaction between elastic waves and dislocations can be found in the literature. Very recently, we have tackled this problem in a bi-dimensional configuration. Firstly, we have considered the problem for the interaction between a single dislocation and an elastic wave (Maurel et al. 2004a). Then, we have studied the properties of a coherent wave (its refraction index and attenuation length) propagating in a medium filled with randomly placed dislocations (Maurel et al. 2004b), the motivation being to extend the ultrasonic non-destructive evaluation for the detection of flaws and cracks to the ultrasonic...
non-destructive evaluation of dislocation ensembles, thus enabling a non-intrusive probe for the study of plasticity.

In this paper, we focus on the two-dimensional multiple scattering process generated by a random distribution of lines that are composed of a line distribution of edge dislocations within an otherwise homogeneous isotropic medium. This is our cartoon of a polycrystal. The paper is organized as follows: in §2, we present the basic relations that lead to an homogeneous wave equation for the in-plane velocity associated with wave displacement:

$$\left[ \nabla^2 + k^2 + (\gamma^2 - 1)\nabla\nabla \right] u(x) = -V_{GB}(x)u(x).$$

Equation (1.1) has a classical form: the left-hand side term corresponds to the usual wave equation whose solutions are two in-plane waves: a transverse wave with a wavevector of modulus $k_\beta$, and a longitudinal wave of modulus $k_\alpha = k_\beta/\gamma$. The right-hand side term describes the interaction between the waves and the grain boundary (i.e. the scatterer) through the potential $V_{GB}$ that has a matrix structure. Then, equation (1.1) is used to determine the scattering functions for a single grain boundary. For in-plane polarized waves, four scattering functions have to be determined. Sections 3 and 4 treat the coherent propagation of waves through multiple grain boundaries (let us remind that these multiple grain boundaries are our cartoon of a polycrystal). In §3, the multiple scattering formalism is presented. Because of the linearity of equation (1.1), the potential $V$ for a grain boundary ensemble, each grain boundary being indexed by $i$, is simply deduced from the potential $V_{GB}^i$ for a single grain boundary through $V = \sum_i V_{GB}^i$. The main task here is to derive the so-called modified, or averaged, Green’s function that is the impulse response of the effective medium, defined as the average of the media over all realizations of grain boundary ensembles. In §4, the characteristics of the coherent wave, in terms of velocity and attenuation, are derived and discussed.

We report in the electronic supplementary material some technical algebra.

2. Scattering mechanism

We recall in this section the main results obtained in Maurel et al. (2004a) to obtain the potential $V^D$ for a scatterer composed of a single dislocation. The potential $V_{GB}$ for a dislocation ensemble is $V_{GB} = \int C dX_i \rho_i(X_i) V^D$, corresponding...
to a line distribution of dislocations with a line density $\rho_b(X_i)$. In the following, we assume this density to be constant [$\rho_b(X_i) = \rho_b$], i.e. we assume the grain boundary is formed of a uniform distribution of dislocations. Note that we could consider $V^G$ as a discrete sum over point dislocations (i.e. a line density made of delta functions); this latter choice being less tractable mathematically.

We consider a two-dimensional space with the fixed basis $(O, e_1, e_2)$. Dislocations are gliding edge dislocations, i.e. their Burgers vectors $b$ are in-plane and their motion, described by the dislocation position $X$, occurs along the Burgers vector $b$. The basis attached to the dislocation is $(t, n)$, with $b = \beta t$ and $n$ along the in-plane perpendicular direction. The two types of in-plane waves interacting with an edge dislocation are: a longitudinal wave with compressional velocity $\alpha = \sqrt{(\lambda + 2\mu)/\rho}$ and a transverse wave with shear velocity $\beta = \sqrt{\mu/\rho}$, where $(\lambda, \mu)$ are Lamé’s constants and $\rho$ the density of the elastic medium. We define $\gamma \equiv \alpha/\beta$, as in equation (1.1).

(a) Potential for a single dislocation

In this section, we want to obtain the potential for a single dislocation. Firstly, equation (2.1) is the starting relation to do that. It corresponds to the integral representation for the particle velocity $v = \dot{u}$ ($u$ is the displacement field in the elastic medium and the dot denotes the time derivative) produced by a moving dislocation located at position $X$. Secondly, equation (2.3) is the equation of motion of a gliding edge dislocation in the presence of an incident wave.

The integral representation

$$v_m(x, t) = \epsilon_{kn} c_{ijkl} \int dt' b_l \dot{X}_n(t') \frac{\partial}{\partial x_j} G^0_{im}(x - X, t - t')$$

is derived from the wave equation

$$\rho \dddot{u}_i(x, t) - c_{ijkl} \frac{\partial^2}{\partial x_j \partial x_k} u_l(x, t) = 0$$

with boundary conditions

$$[u_i]_{S(t)} = b_i, \quad \left[ c_{ijkl} \frac{\partial u_l}{\partial x_k} n_j \right]_{S(t)} = 0,$$

where $S(t)$ is a time-dependent line abutting at the dislocation point (in two-dimensional) and the brackets denote the difference above and below $S(t)$. A derivation of the integral representation has been performed in Mura (1963) and is detailed in electronic supplementary material-1. Similar derivation can be found in Lund (2002) for a vortex loop configuration. In equation (2.1), the indexes $j, k, n...$ take the value 1 or 2, and $\epsilon_{kn} \equiv \epsilon_{kn3}$ (the usual completely antisymmetric tensor). $G^0_{im}(x, t)$ is the elastic Green function in two dimensions.

In the local basis $(t, n)$ introduced earlier, the equation of motion for a gliding edge dislocation reads

$$m \ddot{X}(t) = \tilde{\sigma}_{12} b,$$

where $\tilde{\sigma}_{12}$ is the stress tensor expressed in the local basis $(t, n)$ taken at the position $X(t)$ of the dislocation and where $m$ is the effective mass of an edge.
dislocation

\[
m = \frac{1}{4\pi} \frac{1 + \gamma^4}{\gamma^4} \rho b^2 \ln \frac{\delta}{\delta_0}
\]  

(2.4)

with \( \delta \) and \( \delta_0 \) the long- and short-distance cut-off lengths, respectively.

This equation, valid in the subsonic case (dislocation velocity small compared with \( \alpha, \beta \)), corresponds to an edge dislocation with mass \( m \) submitted to the usual Peach–Koehler force (Peach & Koehler 1950). For the derivation of this equation, see for instance Lund (1988).

Equations (2.1) and (2.3) can be combined into the following wave equation written in the frequency domain (\( \omega \) denotes the frequency and \( k_\beta \equiv \omega/\beta \))

\[
[\nabla^2 + k_\beta^2 + (\gamma^2 - 1) \nabla \nabla_x] \mathbf{v}(x) = -\mathbf{V}^D(x) \mathbf{v}(x),
\]

(2.5)

where the right-hand side of this equation is a two-component vector ‘potential’ given by

\[
\mathbf{V}^D(x) \mathbf{v}(x) = \left( \begin{array}{c} s_t(x) \\ s_n(x) \end{array} \right) = \frac{\mu b^2}{m \omega^2} (\partial_n v_t + \partial_t v_n) X \left( \begin{array}{c} \partial_n \\ \partial_t \end{array} \right) \delta(x - X)
\]

(2.6)

in the local basis (\( t, n \)) and with \( \partial_a v_X \) denoting \( (\partial v/\partial a)(X) \) (\( \partial_t \) represents the space derivative along the tangent \( t \), not to be confused with a time derivative (dot symbol)). A detailed derivation of this equation can be found in electronic supplementary material-2.

Introducing the matrix \( \mathbf{J} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \), one can express the components \( \mathbf{\nabla}^D \) of the operator in the local basis as

\[
\left( \begin{array}{c} s_t(x) \\ s_n(x) \end{array} \right) = -\mathbf{\nabla}^D(x) \left( \begin{array}{c} v_t(x) \\ v_n(x) \end{array} \right), \quad \text{with} \quad \mathbf{\nabla}^D(x) = \frac{\mu b^2}{m \omega^2} \mathbf{J} \mathbf{\nabla} \delta(x - X) \mathbf{\nabla}_X^T \mathbf{J},
\]

where \( \mathbf{\nabla} \equiv \left( \begin{array}{c} \partial_t \\ \partial_n \end{array} \right) \) and \( \mathbf{\nabla}_X^T \) is the operator (acting on any function \( f(x) \)) defined as

\[
\mathbf{\nabla}_X^T f(x) \equiv \left( \begin{array}{c} \partial_t f(X) \\ \partial_n f(X) \end{array} \right). \quad \text{Superscript T denotes the transpose.}
\]

Expressing all quantities in the basis \( (e_1, e_2) \), the operator \( \mathbf{\nabla}^D \) finally reads

\[
\mathbf{\nabla}^D(x) = \frac{\mu b^2}{m \omega^2} \mathbf{R}_{\theta_0} \mathbf{J} \mathbf{\nabla} \delta(x - X) \mathbf{\nabla}_X^T \mathbf{R}_{\theta_0} \mathbf{J}
\]

(2.7)

with \( \theta_0 \equiv (e_1, b) \) and \( \mathbf{R}_a \equiv \begin{pmatrix} \cos a & -\sin a \\ \sin a & \cos a \end{pmatrix} \) the rotation matrix of angle \( a \). We have used \( \mathbf{R}_a \mathbf{J} = \mathbf{J} \mathbf{R}_{-a} \).

(b) ‘Potential’ for a grain boundary

A grain boundary is represented by a segment \( \mathcal{L} \) of length \( L \), containing \( N = \rho_b L \) dislocations (figure 2). The \( N \) dislocations have the same orientation, perpendicular to \( \mathcal{L} \) and the same Burgers vectors \( b \). Possible interactions between dislocations are not considered, except in the term of mass, as
discussed in §3c. The potential $V^{GB}$ associated with the grain boundary is obtained by summing over dislocations

$$V^{GB}(x) = \frac{\mu b^2}{2\Omega} \rho_b \int_{\mathcal{L}} \delta(x - Y) \nabla^T \nabla \delta(x - Y) \rho_b J, \quad (2.8)$$

where $Y = X_c + X$, with $X_c$ an origin point on $\mathcal{L}$ and $X$ oriented along $\mathcal{L}$.

\hspace{1cm}(c) Scattering functions of a single grain boundary

In this section, we derive the scattering functions for a single grain boundary in the first Born approximation. $X_c$ is set equal to $0$ without loss of generality ($Y = X$).

Within the first Born approximation, the integral representation for the solution of equation (2.5) is

$$v^s(x) = \int dx' G^0(x - x', \omega) V^{GB}(x') v^{inc}(x'), \quad (2.9)$$

where $V^p$ has been replaced by the grain boundary potential $V^{GB}$ introduced in equation (2.8), and $v$ has been replaced in the right-hand side term by $v^{inc}$ (the velocity displacement of the incident wave). This assumes weak scattering since the total velocity $v = v^{inc} + v^s$ is assumed to be equal to $v^{inc}$ at leading order (the wave scattered by the rest of the grain boundary on one dislocation is neglected).

In the case of polarized waves, one has to distinguish the amplitudes $A_\alpha$ and $A_\beta$ of the longitudinal and transverse incident waves, respectively:

$$v^{inc}(x) = A_\alpha e_1 e^{ik_x x_1} + A_\beta e_2 e^{ik_y x_1}. \quad (2.10)$$

The incident wave propagates along the $e_1$-axis, so that the velocity of the longitudinal wave is along $e_1$ and the velocity of the transverse wave is along $e_2$ (figure 3). In the following, $v^\alpha(x)$ [$v^\beta(x)$] denotes the solution of equations (2.9) and (2.10) with $A_\beta = 0$ ($A_\alpha = 0$, respectively).

Because equation (2.9) is linear, the full solution is simply the superposition $v^s = v^\alpha + v^\beta$. We present in the following the detailed derivation of the scattered wave $v^\beta(x)$. The derivation of $v^\alpha(x)$ is performed in a similar way.

We first express the components of $v^\beta(x)$ (respectively, $v^\alpha(x)$) in cylindrical components: the first component corresponds to the projection of $v^\beta(x)$ along...
Figure 3. Scattering of an incident wave with longitudinal and transverse polarizations \((A_{\alpha} \text{ and } A_{\beta}, \text{ respectively})\) by a grain boundary \(L\). At an observation angle \(\theta\) and at large distances \(x\) from \(L\), the scattered field is composed of a longitudinal wave (with scattering functions \(f_{\alpha\alpha}\) and \(f_{\beta\beta}\) because of mode conversion) and of a transverse wave (with scattering functions \(f_{\alpha\beta}\) and \(f_{\beta\alpha}\)).

The position vector \(x\), with \(\theta \equiv (e_1, x)\) and the second component is the azimuthal component. In this local basis, we use two remarkable properties: (i) the Green function \(\hat{G}(x, \omega)\), defined by \(G^0_{ij}(x, \omega) = R_{ij,0} \hat{G}_{ij}(x, \omega) R_{ij,0}\), is diagonal and independent of \(\theta\) (\(x\) denotes the magnitude of the position vector \(x\)); (ii) the polar components of \(v^s\) are directly related to the scattering functions \(f_{\alpha\alpha}(\theta)\) and \(f_{\beta\beta}(\theta)\). In these notations, \(f_{\alpha\beta}(\theta)\) is the \(a\)-component of the scattered wave, for a given incident \(b\)-wave. That is, in the limit \(kx \gg 1\),

\[
\begin{pmatrix}
    v_{\alpha, t}^s \\
    v_{\alpha, n}^s
\end{pmatrix} = A_{\alpha} \begin{pmatrix}
    f_{\alpha\alpha}(\theta) \frac{e^{ik_{\alpha}x}}{\sqrt{x}} \\
    f_{\beta\alpha}(\theta) \frac{e^{ik_{\beta}x}}{\sqrt{x}}
\end{pmatrix}, \quad \text{resp.} \quad \begin{pmatrix}
    v_{\beta, t}^s \\
    v_{\beta, n}^s
\end{pmatrix} = A_{\beta} \begin{pmatrix}
    f_{\alpha\beta}(\theta) \frac{e^{ik_{\alpha}x}}{\sqrt{x}} \\
    f_{\beta\beta}(\theta) \frac{e^{ik_{\beta}x}}{\sqrt{x}}
\end{pmatrix},
\]

(2.11)

The scattering functions \(f_{\beta\alpha}\) and \(f_{\alpha\beta}\) quantify mode conversions, i.e. the transverse wave generated from scattering of a longitudinal incident wave, and vice versa.

Using equation (2.8) and setting \(A_{\beta} = 0\), \(A_{\alpha} = 1\), the integral representation (2.9) reads

\[
v_{\alpha}^s(x) = \frac{\rho_b \mu_b \gamma}{m \omega^2} \int d x' \int_\mathcal{L} dX' G^0(x - x', \omega) R_{2\theta_0} J \nabla' \delta(x' - X) \nabla_{x}|_X^T R_{2\theta_0} J e_1 e^{i k_{\alpha} x'}. \quad (2.12)
\]

In the integral above, we have

\[
\nabla_{x}|_X^T R_{2\theta_0} J e_1 e^{i k_{\alpha} x'_1} = i k_{\alpha} e_1 |_{2\theta_0}^T R_{2\theta_0} J e_1 e^{i k_{\alpha} X_1} = -i k_{\alpha} \sin 2 \theta_0 \ e^{i k_{\alpha} X_1}, \quad (2.13)
\]

and the integral over \(x'\) is

\[
\left(\int d x' G^0(x - x', \omega) R_{2\theta_0} J \nabla' \delta(x' - X)\right)^T = \nabla^T R_{2\theta_0} J G^0(x - X, \omega). \quad (2.14)
\]
We now use, for \( x \gg X \) (where \( X \) denote the magnitude of the position vectors \( x, X \)), the asymptotic form of Green’s function in two-dimensional free space

\[
C^0(x - X, \omega) \xrightarrow{x \to \infty} \frac{e^{i\pi/4}}{2\sqrt{2\pi\alpha}} R_\theta \begin{pmatrix}
\frac{e^{ik_x|x + X\sin(\theta_0 - \theta)|}}{\sqrt{k_x}} & 0 \\
0 & \frac{e^{ik_x|x + X\sin(\theta_0 - \theta)|}}{\sqrt{k_x}}
\end{pmatrix} R_{-\theta}.
\]

(2.15)

We have used \( X = XR_{\theta_0}e_2 \): with \( X_c = 0 \), \( X \) is along the direction of the dislocation line, perpendicular to the Burgers vector \( b \) along \( R_{\theta_0}e_1 \).

In general, \( \nabla = \partial_x (R_\theta e_1) + (1/x)\partial_\omega (R_\theta e_2) \). At leading order in \( x \), the terms coming from the derivation with respect to \( \omega \) can be neglected, so that we formally write \( \nabla = R_{\theta}\partial_x e_1 \) that involves the leading order terms. We get for the cylindrical components

\[
\begin{pmatrix}
\mathbf{v}_{\alpha,c}^s(x) \\
\mathbf{v}_{\alpha,n}^s(x)
\end{pmatrix} = R_{-\theta} \begin{pmatrix}
\mathbf{v}_{\alpha,1}^s(x) \\
\mathbf{v}_{\alpha,2}^s(x)
\end{pmatrix}
\]

\[
= \frac{\rho_{\theta}\mu b^2}{m\omega^2} \frac{e^{i\pi/4}}{2\sqrt{2\pi|x|}} \sin 2\theta_0 k_x \int_L dX e^{ik_x X_i} \begin{pmatrix}
\frac{\sqrt{k_x}}{\gamma^2} e^{ik_x|x + X\sin(\theta_0 - \theta)|}\sin 2(\theta - \theta_0) \\
\sqrt{k_x} e^{ik_x|x + X\sin(\theta_0 - \theta)|}\cos 2(\theta - \theta_0)
\end{pmatrix},
\]

where we have used \( R_{2\theta_0 - \theta}JR_{\theta}e_1 = \begin{pmatrix} \sin 2(\theta - \theta_0) \\ \cos 2(\theta - \theta_0) \end{pmatrix} \). We finally obtain

\[
\begin{pmatrix}
\mathbf{v}_{\alpha,c}^s(x) \\
\mathbf{v}_{\alpha,n}^s(x)
\end{pmatrix} = \frac{\mu Nb^2}{m\omega^2} \frac{e^{i\pi/4}}{2\sqrt{2\pi|x|}} \sin 2\theta_0 k_x
\]

\[
\times \begin{pmatrix}
\frac{\sqrt{k_x}}{\gamma^2} e^{ik_x}\sin\{k_x L/[2(\sin(\theta_0 - \theta) - \sin \theta_0)]\}\sin 2(\theta - \theta_0) \\
\sqrt{k_x} e^{ik_x}\sin\{k_x L/[2(\sin(\theta_0 - \theta) - \sin \theta_0)]\}\cos 2(\theta - \theta_0)
\end{pmatrix}.
\]

(2.16)

The case of the transverse incident wave can be treated using the same route as in \$2a\): In equation (2.12), the term \( \nabla x^T_{X} R_{2\theta_0}J e_1 e^{ik_x x^t} = -ik_x \sin 2\theta_0 e^{ik_x X_1} \) has to be replaced by \( \nabla x^T_{X} R_{2\theta_0}J e_2 e^{ik_x x^t} = ik_x \cos 2\theta_0 e^{ik_x X_1} \). We deduce

\[
\begin{pmatrix}
\mathbf{v}_{\beta,c}^s(x) \\
\mathbf{v}_{\beta,n}^s(x)
\end{pmatrix} = -\frac{\mu Nb^2}{m\omega^2} \frac{e^{i\pi/4}}{2\sqrt{2\pi|x|}} \cos 2\theta_0 k_x
\]

\[
\times \begin{pmatrix}
\frac{\sqrt{k_x}}{\gamma^2} e^{ik_x}\sin\{k_x L/[2(\sin(\theta_0 - \theta) - \gamma \sin \theta_0)]\}\sin 2(\theta - \theta_0) \\
\sqrt{k_x} e^{ik_x}\sin\{k_x L/[2(\sin(\theta_0 - \theta) - \gamma \sin \theta_0)]\}\cos 2(\theta - \theta_0)
\end{pmatrix}.
\]

(2.17)
Elastic wave propagation in polycrystals

The scattering functions are then written by identifying equations (2.16) and (2.17) with equation (2.11)

\[
\begin{align*}
 f_{\alpha\alpha}(\theta) &= \frac{\mu Nb^2}{18m\omega^2} \frac{k^{3/2}_\alpha}{2\sqrt{2\pi}} \sin 2\theta_0 \sin 2(\theta - \theta_0) \sin 2(\theta_0 - \theta) \sin[ k_\alpha L / 2(\sin(\theta_0 - \theta) - \sin \theta_0)] e^{i\pi/4}, \\
 f_{\beta\alpha}(\theta) &= \frac{\mu Nb^2}{18m\omega^2} \frac{k^{1/2}_\alpha k^{1/2}_\beta}{2\sqrt{2\pi}} \sin 2\theta_0 \cos 2(\theta - \theta_0) \sin 2(\theta_0 - \theta) \sin[ k_\beta L / 2(\sin(\theta_0 - \theta) - \sin \theta_0 / \gamma)] e^{i\pi/4}, \\
 f_{\alpha\beta}(\theta) &= \frac{-\mu Nb^2}{18m\omega^2} \frac{k^{1/2}_\alpha k^{1/2}_\beta}{2\sqrt{2\pi}} \cos 2\theta_0 \sin 2(\theta - \theta_0) \sin 2(\theta_0 - \theta) \sin[ k_\alpha L / 2(\sin(\theta_0 - \theta) - \gamma \sin \theta_0)] e^{i\pi/4}, \\
 f_{\beta\beta}(\theta) &= \frac{-\mu Nb^2}{18m\omega^2} \frac{k^{3/2}_\beta}{2\sqrt{2\pi}} \cos 2\theta_0 \cos 2(\theta - \theta_0) \sin 2(\theta_0 - \theta) \sin[ k_\beta L / 2(\sin(\theta_0 - \theta) - \sin \theta_0)] e^{i\pi/4}. 
\end{align*}
\]

(2.18)

The polar plots of the scattering functions are shown in figure 4. As expected, for wavelengths large compared to \( L \), the scattering functions tend to those
obtained for a single dislocation with Burgers vector $\mathbf{B} \equiv Nb$ and mass $M \equiv Nm$ (see Maurel et al. 2004a).

3. The multiple scattering mechanism for the modified Green function

(a) Principle of the calculation

The multiple scattering formalism we use is based on the calculation of the modified Green function $\langle \mathbf{G} \rangle (k)$ with $k$ the wavevector that comes from the Fourier transform of $G(\mathbf{x})$. The modified Green function describes the elastic medium filled with scatterers randomly distributed (here, the segments $L$ representing grain boundaries) in terms of an effective medium. The averaging process over disorder realizations involves averages over the lengths $L$ of the segments, over the dislocations densities $\rho_b = 1/d$ held by each segment ($d$ denotes the distance between two dislocations), over the Burgers vectors $\mathbf{b}$ of the $N = \rho_b L$ dislocations held by the segments, and over the positions and orientations of the segments $(\mathbf{X}_c, \theta_0)$ (figure 2). The modified Green function is given by the Dyson equation (see, for instance, Sheng 1995)

$$\langle \mathbf{G} \rangle (k) = \left[ \mathbf{G}^0 (k) - \sum (k) \right]^{-1},$$

where $\mathbf{G}^0$ is the free space Green function and $\sum (k)$ the so-called mass operator. When the properties of the coherent wave differ little from the waves in the homogeneous medium, $\sum (k)$ can be perturbatively expanded in powers of a small parameter $\epsilon$ (for a discussion/definition of $\epsilon$, see §3c): $\sum (k) = \sum_1 (k) + \sum_2 (k) + \cdots$. In the present case, we need to compute at least the first two terms, because the imaginary part of the leading term $\sum_1 (k)$ vanishes. These terms are given by

$$\sum_1 (k) = n \int d\mathbf{x} \, d\mathbf{C} \, e^{-ik \cdot \mathbf{x}} \mathbf{V}^\text{GB} (\mathbf{x}) e^{ik \cdot \mathbf{x}},$$

$$\sum_2 (k) = n \int d\mathbf{x} \, d\mathbf{x'} \, d\mathbf{C} \, e^{-ik \cdot \mathbf{x}} \mathbf{V}^\text{GB} (\mathbf{x}) \mathbf{G}^0 (\mathbf{x-x'}) \mathbf{V}^\text{GB} (\mathbf{x'}) e^{ik \cdot \mathbf{x'}},$$

where $n$ denotes the number density of scatterers (grain boundaries) per unit area and the integral over $\mathbf{C}$ corresponds to averages over all relevant parameters. Here, $d\mathbf{C} = p(b) dbp(L) dLp(\rho_b) d\rho_b (d\mathbf{X}_c / V)(d\theta_0 / 2\pi)$, where $p(X)$ denotes the probability distribution function of the quantity $X$ (in the following, we note $\langle X \rangle = \int dXXp(X)$). In equation (3.2), we have assumed that the scatterers are not spatially correlated.

The (complex) poles of $\langle \mathbf{G} \rangle (k)$ give the wavenumbers $K_x$ and $K_y$ of the coherent waves that can propagate in the effective medium. Their real part is related to the index of refraction whereas their imaginary part is related to the attenuation length.

We report in §3b the derivation of $\sum (k)$ at order 1. The derivation at order 2, that involves similar calculations, is detailed in electronic supplementary material-3.
(b) Derivation of the mass operator

(i) Order 1

We start from the expression (3.2) for $\sum_1(k)$

$$\sum_1(k) = n \int \mathrm{d}x \ p(b)p(L)p(\rho_b) \mathrm{d}L \frac{\mathrm{d}\theta_0}{2\pi} \frac{\mathrm{d}X_r}{V} e^{-i k \cdot x} V_{GB}(x) e^{i k \cdot x}. \quad (3.3)$$

Using equation (2.8), we get

$$\sum_1(k) = n \frac{\mu}{\omega^2} \left\langle \frac{\rho_b b^2}{m} \right\rangle \int \mathrm{d}x p(L) \frac{\mathrm{d}L}{2\pi} \frac{\mathrm{d}X_r}{V}$$

$$\times \int_L \mathrm{d}X e^{-i k \cdot x} R_{2\theta_0} J \nabla \delta(x - Y) \nabla_{|Y}^{T} R_{2\theta_0} J e^{i k \cdot x}.$$

By using $\nabla_{|Y}^{T} e^{i k \cdot x} = i k^T e^{i k \cdot Y}$ and integrating by part $\int \mathrm{d}x e^{-i k \cdot x} \nabla \delta(x - Y) = i k e^{-i k \cdot Y}$, we obtain

$$\sum_1(k) = -n \frac{\mu}{\omega^2} \left\langle \frac{\rho_b b^2}{m} \right\rangle \int p(L) \frac{\mathrm{d}L}{2\pi} \frac{\mathrm{d}X_r}{V} \int_L \mathrm{d}X r_{2\theta_0} J k^T k R_{2\theta_0} J.$$

We now focus on the matrix $R_{2\theta_0} J k^T k R_{2\theta_0} J$ whose average over $\theta_0$ has to be taken. With $k = k R_{2\theta_0} e_1$ (i.e. $\xi = (e_1, k)$), and using $P_1 \equiv e_1^T e_1$ and $P_2 \equiv e_2^T e_2 = J P_1 J$, it is easy to see that $R_{2\theta_0} J k^T k R_{2\theta_0} J = k^2 R_{(2\theta_0 - \tilde{\xi})} J P_2 R_{-(2\theta_0 - \tilde{\xi})}$. Changing the variable $\theta_0 \rightarrow \theta_0 - \xi / 2$, we obtain

$$\sum_1(k) = -n \frac{\mu}{2\pi \omega^2} \left\langle \frac{N b^2}{m} \right\rangle k^2 \int \mathrm{d}\theta_0 P_{2\theta_0} P_{2\theta_0}$$

$$= -n \frac{\mu}{2\omega^2} \left\langle \frac{N b^2}{m} \right\rangle k^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (3.5)$$

For a single grain boundary, the total Burgers vector is $B \equiv Nb$ and the total mass is $M \equiv Nm$. Expression (3.5) is actually the same as obtained for a random distribution of isolated dislocations of Burgers vector $B$ and mass $M$ (Maurel et al. 2004b)

$$\sum_1(k) = -\frac{1}{2} \frac{\mu n}{\omega^2} \left\langle \frac{B^2}{M} \right\rangle k^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (3.6)$$

This result shows that there is no effect of the line distribution of dislocations along the segments $\mathcal{L}$ at this order: grain boundaries are seen as spatially uncorrelated (‘fat’) single dislocations.
(ii) **Order 2**

The calculation of $\sum_2(k)$ is similar to that presented earlier and is detailed in the electronic supplementary material-3. We obtain

$$\sum_2(k) = \frac{i}{16} \left( \frac{\mu n}{\omega^2} \right)^2 \left\langle \frac{N^2 b^4}{m^2} \right\rangle \left( 1 + \frac{\gamma^4 k^2}{\gamma^4 n} \right) R_\gamma \begin{pmatrix} I_1(kL) & 0 \\ 0 & I_2(kL) \end{pmatrix} R_{-\gamma}$$

(3.7)

with

$$I_1(kL) = \frac{1}{\pi^2(L^2)(1 + \gamma^4)} \int p(L) L^2 \, dL \, d\theta_0 \, d\zeta \sin^2 \theta_0$$

$$\times \{ \cos^2 2\zeta f(k_a L, kL, \theta_0, \zeta) + \gamma^4 \sin^2 2\zeta f(k_\beta L, kL, \theta_0, \zeta) \},$$

$$I_2(kL) = \frac{1}{\pi^2(L^2)(1 + \gamma^4)} \int p(L) L^2 \, dL \, d\theta_0 \, d\zeta \cos^2 \theta_0$$

$$\times \{ \cos^2 2\zeta f(k_a L, kL, \theta_0, \zeta) + \gamma^4 \sin^2 2\zeta f(k_\beta L, kL, \theta_0, \zeta) \}$$

and

$$f(qL, kL, \theta_0, \zeta) = \text{sinc}^2[(k \sin \theta_0 - q \sin \zeta)L/2],$$

where $\text{sinc}(x) \equiv \sin(x)/x$. It is easy to see that $I_{a=1,2}$ goes to unity as $kL$ tends to zero. Hence, the limit of expression (3.7) at long wavelengths is the same as that obtained for a random distribution of single dislocations of Burgers vector $B$ and mass $M$

$$\sum_2(k) = \frac{i}{16} \left( \frac{\mu n}{\omega^2} \right)^2 \left\langle \frac{B^4}{M^2} \right\rangle \left( 1 + \frac{\gamma^4 k^2}{\gamma^4 n} \right) R_\gamma \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$  

(3.8)

Using

$$G^0(k) = R_\gamma \begin{pmatrix} \gamma^2 (k^2 - k_\alpha^2) & 0 \\ 0 & (k^2 - k_\beta^2) \end{pmatrix} R_{-\gamma}$$

(3.9)

the modified Green function finally reads

$$\langle G \rangle^{-1}(k) = R_\gamma \left[ \begin{pmatrix} \gamma^2 (k^2 - k_\alpha^2) & 0 \\ 0 & k^2 - k_\beta^2 \end{pmatrix} + \frac{1}{2} \frac{\mu n}{\omega^2} \left\langle \frac{B^2}{M} \right\rangle k^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] R_{-\gamma}.$$  

(3.10)

(c) **Discussion**

Let us comment on expression (3.10). For the sake of clarity, we take all grain boundaries with the same number of dislocations, so that $N^2 = \langle N \rangle^2 = \langle N \rangle^2$. 

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Relation (2.4) can be written as \( m = \rho b^2 / \epsilon \), where \( \epsilon \equiv 1 / \ln(\delta / \delta_0) \) is the small parameter in multiple scattering by single dislocations. We have \( B^2 / M = \eta / \rho \) and we define

\[
\epsilon' \equiv \frac{n}{k_\beta^2},
\]

so that we can write, for \( k = ke_1 \) (i.e. \( \xi = 0 \))

\[
\langle G \rangle^{-1}(k) = G_0^{-1}(k)
\]

\[
+ \epsilon' k^2 \left[ \frac{1}{2} N \epsilon \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \frac{i}{16} \frac{1 + \gamma^4}{\gamma^4} (N \epsilon)^2 \begin{pmatrix} I_1(kL) & 0 \\ 0 & I_2(kL) \end{pmatrix} \right].
\]

The weak scattering limit corresponds to

(i) \( \epsilon' \) finite, that is no vanishing value of \( k_\beta L_c \), with \( L_c \approx 1 / \sqrt{n} \);

(ii) \( N \epsilon \ll 1 \), with \( \epsilon \approx 1 / \ln(\delta / \delta_0) \).

The first condition introduces a cut-off length \( L_c \) for the ultrasonic wavelength that can be used. As the interaction strength between the wave and a dislocation increases with increasing wavelength, this condition corresponds to a non-divergence of the scattering strength. This condition introduces a characteristic length that is relevant in the forthcoming expressions of the refraction indices (4.2) and of the attenuation lengths (4.4). Note that in a recent experiment (Zolotoyabko et al. 2001; Shilo & Zolotoyabko 2002, 2003), high frequency ultrasonic waves have been used in a LiNbO\(_3\) crystal, corresponding to \( k_\beta L_c \approx 10 \), thus fulfilling condition (i).

Condition (ii) involves properties of the medium itself. For an isolated dislocation, the long cut-off length \( \delta \) is given by the size of the sample and the short cut-off length \( \delta_0 \approx b \). In grain boundaries, the upper cut-off length \( \delta \) can be chosen as the distance \( d \) between dislocations (Shockley & Read 1949). For a tilt boundary, \( L, N \) and \( b \) are linked through \( L = Nd \), with \( d = b / \theta_b \) and \( \theta_b \) the (small) misorientation angle. We thus obtain the condition

\[
N \epsilon = \frac{(L/b)}{\ln(d/b)} \theta_b \ll 1.
\]

With \( L \gg b \), this condition gives a restriction on the angle \( \theta_b \) of the grain boundary.

4. Characteristics of the coherent waves

The wavenumbers \( K_\alpha \) and \( K_\beta \) of the coherent longitudinal and transverse waves, respectively, are given by the poles of \( \langle G \rangle(k) \). In equation (3.10), the first diagonal term of \( \langle G \rangle^{-1}(k) \) gives the longitudinal wave (directed along \( k \));

the second diagonal term yields the transverse wave, in the direction perpendicular to \( k \). In the weak scattering approximation, \( K_\alpha \) is expected to be close to \( k_\alpha \) (and \( K_\beta \) close to \( k_\beta \)). In equation (3.10), we thus replace \( I_1(kL) \) by
\( I_1(k_L) \) (and \( I_2(kL) \) by \( I_2(kbL) \)). Thus, the coherent wavenumbers read

\[
K_\alpha = k_\alpha \left[ 1 - \frac{\mu n}{4 \gamma^2 \omega^2} \left( \frac{N b^4}{m} \right) + \frac{1}{n} \frac{\alpha}{\gamma} \left( \frac{N b^4}{m^2} \right) \right] \left[ k_\alpha^2 \frac{I_1(k_\alpha L)}{n} \right],
\]

\[
K_\beta = k_\beta \left[ 1 - \frac{\mu n}{4 \omega^2} \left( \frac{N b^4}{m} \right) + \frac{1}{n} \frac{\beta}{\gamma} \left( \frac{N b^4}{m^2} \right) \right] \left[ k_\beta^2 \frac{I_2(k_\beta L)}{n} \right].
\]

At first-order, this expression reduces to the results obtained following Foldy’s approach (see §4c).

(a) Index of refraction and attenuation length

We define the index of refraction as \( n_\alpha \equiv \alpha/V_\alpha \) (respectively, \( n_\beta \equiv \beta/V_\beta \)), where \( V_\alpha = \text{Re}(\omega/K_\alpha) \) denote the phase velocities in the presence of grain boundaries (remind that \( \alpha \) and \( \beta \) are the phase velocities in the absence of grain boundaries). From equation (4.1), we obtain

\[
n_\alpha = 1 - \frac{1}{4 \gamma^2 \omega^2} \frac{\mu n}{m} \left( \frac{N b^4}{m} \right),
\]

\[
n_\beta = 1 - \frac{1}{4 \omega^2} \frac{\mu n}{m} \left( \frac{N b^4}{m} \right).
\]

As observed for a distribution of isolated dislocations (Maurel et al. 2004b):

(i) the effective phase velocity is larger than its value in the absence of scatterers. The group velocity is however smaller;

(ii) the index of refraction decreases with increasing wavelength.

As first observed by Nabarro (1951) and confirmed in our calculations, this result is due to the particular interaction between an elastic wave and a dislocation (e.g. in equation (2.3)). The scattering waves actually occur from the motion of the dislocation driven by the incident wave. The equation of motion (Lund 1988) shows that the amplitude of dislocation motion increases with increasing wavelengths, which also increases the scattered energy. Of course, no divergence of the index occurs since the difference of \( n_\alpha, n_\beta \) to unity is of order \( N c \epsilon' \). With the condition that \( \epsilon' \) remains finite, values of wavelengths have an upper limit given by the cut-off length \( L_c \). By considering identical grain boundaries, equation (4.2) reads

\[
n_\alpha = 1 - \frac{1}{4 \gamma^2 \omega^2} \frac{\mu n b^2}{M \omega^2} = 1 - \frac{1}{4 \gamma^2 \omega^2} \frac{N c}{(k_\alpha L_c)^2},
\]

\[
n_\beta = 1 - \frac{1}{4 \omega^2} \frac{\mu n b^2}{M \omega^2} = 1 - \frac{1}{4 \omega^2} \frac{N c}{(k_\beta L_c)^2}.
\]

(b) Attenuation lengths

The attenuation length \( \Lambda_a \) is given by the imaginary part of the wavenumber: \( \Lambda_a \equiv 1/\text{Im}(K_a) \). It corresponds to the loss of coherence due to scattering away
from the forward direction. From equation (4.1), we obtain

\[
A_\alpha = \frac{32\gamma^4 \alpha^4}{1 + \gamma^4 \mu^2} \left< \frac{m^2}{N^2b_1^4} \right> \frac{k_\alpha}{I_1(k_\alpha L)} \sim \frac{32\gamma^8}{1 + \gamma^4} \frac{1}{(N\epsilon)^4} \frac{k_\alpha L_c}{I_1(k_\alpha L)} L_c,
\]

\[
A_\beta = \frac{32\gamma^4 \beta^4}{1 + \gamma^4 \mu^2} \left< \frac{m^2}{N^2b_1^4} \right> \frac{k_\beta}{I_2(k_\beta L)} \sim \frac{32\gamma^8}{1 + \gamma^4} \frac{1}{(N\epsilon)^4} \frac{k_\beta L_c}{I_2(k_\beta L)} L_c,
\]

where the symbol ‘\(\sim\)’ can be replaced by an equality if all grain boundaries are identical. The attenuation lengths are plotted in figure 5 as a function of wavenumber. Note the presence of a linear and a quadratic regime, with a crossover between both behaviours occurring at wavelengths of the order of the average grain boundary length. The linear regime coincides with the results obtained with single dislocations (Maurel et al. 2004) with the total Burgers vector \(B\) and the total mass \(M\). Increasing the wavelength decreases the attenuation length \(A_{\alpha,\beta}\), an unusual behaviour for waves propagating in random media. Reversely, waves do not attenuate at very small wavelengths (as the refraction index tends to one), a limit where the medium looks as if disorder-free. Recall that the expressions in equation (4.4) are not valid for large wavenumbers because of the condition that \(\epsilon'\) remains finite.

Note also that, in the calculation presented here, the internal damping has been neglected in the equation of motion. Sources of dislocation damping can be multiple (Nabarro 1987), and are important at low frequencies. In spite of this limitation, the predictions discussed earlier could be further tested experimentally in a frequency range where damping forces are still small.

(c) Remark on the Foldy approach

An adaptation of the Foldy approach (Foldy 1945) can be found in Maurel et al. (2004b) for two-dimensional polarized waves. It was found, for an ensemble

Figure 5. Variations of \(A_\alpha, A_\beta\) (with \(\gamma=1.4\)) as a function of \(k_\beta(L)\). The bold lines represent \(A_\alpha\), with a grain boundary length distribution given by \(p(L) \propto \delta(L-\langle L \rangle)\) (solid line) and \(p(L) = 1/(2\langle L \rangle)\) (dashed line). The thin lines represent \(A_\beta\), with the same notations. The straight dashed lines are guides to the eye.
of isolated dislocations, that \( \langle f_{a|b} \rangle C(0) = \langle f_{b|a} \rangle C(0) = 0 \) (in that case, we had \( C = (b, \theta_0) \)). This property, that is the averaged cross-coupled scattered waves vanish, is also verified for the present case. Indeed, it can be seen from equation (2.18) that the average over \( \theta_0 \) makes \( \langle f_{a|b} \rangle C(\theta) \) and \( \langle f_{b|a} \rangle C(\theta) \) (here, we have \( C = (b, L, \rho_b, X_c, \theta_0) \)) to vanish at \( \theta = 0 \).

Thus, the effective wavenumber \( K_a \), with \( a = \alpha, \beta \), can be written as a function of the averaged scattering functions

\[
K_a = k_a + n \sqrt{\frac{2\pi}{k_a}} \langle f_{aa} \rangle C(0)e^{-i\pi/4}.
\]

This relation leads to the same value for the modified wavenumber as in equation (4.1) at first-order. This is because the scattering functions have been calculated in the first Born approximation.

### 5. Concluding remarks

We have derived the dispersion relation of a two-dimensional continuous elastic medium filled with gliding edge dislocation arrays randomly distributed and oriented in space. It has been found that sound attenuation increases with wavelength, an effect probably due to the two-dimensional nature of the problem.

The present analysis is aimed to evaluate the plastic contribution to the multiple scattering of elastic waves that propagate through polycrystals and it is the first time, to the best of our knowledge, that the structure at the grain boundary is considered. Most of the studies have considered the variations between grains in the elastic constants, and mainly the change in anisotropy, as the source of scattering. Both effects may superpose in polycrystals, so including possible contribution of the dislocations could be helpful to obtain a better modelling of sound propagation in polycrystals.

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### References


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