

# Rigid perfectly plastic two-dimensional polycrystals

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*Received 28 November 2000; revised 24 March 2001; accepted 10 April 2001*

We consider rigid perfectly plastic polycrystals in the two-dimensional anti-plane shear context. The yield sets of the grains are identified with rectangles in the plane centred at the origin whose sides have length 2 and  $2M$ . The limit  $M \rightarrow \infty$  corresponds to the grains being rigid in one direction and ductile in the orthogonal direction.

We show that for large values of  $M$  there exist polycrystals whose effective yield sets are large in all directions. More precisely, for each value of  $M$ , we construct a polycrystal whose yield set contains the set  $[-f, f] \times [-f, f]$ , where  $f = \sqrt{M} - O(1)$ .

We also show that the yield set of any isotropic polycrystal is contained in the ball of radius  $4\sqrt{M}/\pi$  centred at the origin. This bound results as an application of the div-curl lemma. The new component of our analysis, which allowed us to obtain sharper results, is that we consider simultaneously not only two but an infinite number of admissible stress fields whose averages have different directions.

**Keywords:** plasticity; polycrystals; effective behaviour; homogenization

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## 1. Introduction

Metals are usually found in the form of polycrystals, that is, large collections of bonded grains. The atoms of each grain form a periodic lattice and, thus, each grain is a single crystal. A direct consequence of the periodicity of the atomic lattice is that single crystals are generally anisotropic. Thus, the behaviour of polycrystals depends not only on the material properties of the grains, but also on the polycrystalline texture (i.e. shape, orientation and spatial distribution of the grains).

The growth of single crystals is generally expensive and difficult, consequently, in most applications, crystalline materials are used in polycrystalline form. The behaviour of polycrystals may differ substantially from that of the corresponding single crystal. Any isotropic polycrystal whose grains are highly anisotropic is a good example. Furthermore, polycrystals made of the same material but with different texture may also exhibit different behaviour. Since the texture can be partly controlled by processing the material, it is valuable to predict the dependence of the behaviour of polycrystals on their texture to provide guidelines for material selection and processing.

The mathematical modelling of polycrystalline metals is a complex task. Much effort is being devoted to simulate the behaviour of metals numerically. These simulations are usually based on models that take into account several physical effects, such

as plastic and elastic deformations, work hardening, strain ageing, etc. The number of publications in this field is large; two review papers are Dawson & Marin (1997) and Sevillano *et al.* (1981). The complexity of these models forces some approximations to be made. Most notably, the condition of equilibrium is usually replaced by a simpler estimate. Among these estimates the most widely used is the one due to Taylor (1938), which consists of assuming that the strain rate is constant throughout the polycrystal.

Several other schemes to estimate the macroscopic response of nonlinear composite materials (in particular, polycrystalline metals), without directly solving the equilibrium equations, have been developed. The estimate introduced by Sachs (1928) is the result of assuming that the stress is constant throughout the material. Bishop & Hill (1951) showed that the Taylor and Sachs estimates provide bounds (in a sense to be discussed later) of the material behaviour. Hutchinson (1976) introduced self-consistent estimates for power law materials. Willis (1983) and Talbot & Willis (1985) developed a nonlinear version of the Hashin–Shtrikman (Hashin & Shtrikman 1962*a, b*, 1963) variational procedure. A method based on comparing the nonlinear material with an appropriately chosen linear heterogeneous material was created by Ponte Castañeda (1991) and Suquet (1993). Ponte Castañeda (1996) also introduced a method for nonlinear composites that is second order in the contrast of the properties of the phases. A recent review of some of these methods is given in Ponte Castañeda & Suquet (1997). Applications of these methods to rigid-plastic composites can be found in Olson (1994), and to polycrystals whose grains' behaviour are governed by power law creep in Dendievel *et al.* (1991) and deBotton & Ponte Castañeda (1995).

The accuracy of the above-mentioned approximations is uncertain. Since rigid perfectly plastic polycrystals are amenable to deep mathematical analysis and retain the important effects of nonlinearity and those associated with texture, they are ideal materials to test the existing schemes, develop new ones and gain intuition on the behaviour of real materials.

The behaviour of a rigid perfectly plastic single crystal is characterized by a closed convex set  $K$  in the space of stresses (i.e. symmetric  $3 \times 3$  real matrices). This idealized material can only withstand stresses in  $K$ . If the material is subject to a stress  $\sigma$  which is in the interior of  $K$ , it does not deform. On the other hand, if  $\sigma \in \partial K$  (the boundary of  $K$ ), plastic flow occurs (i.e. the material will deform at a certain strain rate).  $K$  is called the yield set.

In the present work we consider rigid perfectly plastic polycrystals in the two-dimensional anti-plane shear context. In §2 we review the equations that describe the behaviour of these polycrystals. The yield set of each grain is identified with a rectangle in the plane centred at the origin. Since the grains are made of the same material, their yield sets have the same dimensions. One set of sides has length 2 and the orthogonal sides have length  $2M$ . On the other hand, the orientation of each yield set is determined by the texture and, thus, it may vary from grain to grain. We assume that the size of the grains is much smaller than the size of the polycrystal that contains them. In this limit, the polycrystal behaves as a rigid perfectly plastic material. The goal is to predict the effective yield set of any given polycrystal. For future reference, we will denote this set by  $K_{\text{hom}}$ .

This problem was first introduced by Kohn & Little (1998). They noted that, for statistically isotropic polycrystals (i.e. every orientation occurs with equal probabilit-

ity), the Sachs and Taylor bounds predict the yield set of the polycrystal to be the balls (centred at the origin) of radius 1 and  $2(M + 1)/\pi$ , respectively. These two approximations differ substantially as  $M$  becomes large and, thus, it is not clear how well they approximate  $K_{\text{hom}}$ . The Sachs bound predicts that the material is ductile in every direction (i.e. its yield set remains bounded) independently of the value of  $M$ . On the other hand, the Taylor bound predicts that the material becomes rigid in every direction as  $M \rightarrow \infty$ .

Kohn & Little (1998) constructed a checkerboard polycrystal whose yield set does not depend on  $M$ . In other words, they showed that there exist polycrystals that remain ductile in every direction independently of the value of  $M$ . However, they left open the question of the existence of polycrystals that become rigid in every direction as  $M \rightarrow \infty$ . In fact, they posed this question. In §3 we show that for large values of  $M$  there exist polycrystals whose effective yield sets are large in all directions. More precisely, for each value of  $M$ , we construct a polycrystal whose yield set contains the set  $[-f, f] \times [-f, f]$ , where  $f = \sqrt{M} - O(1)$ .

Following ideas from the translation method (see, for example, Milton 1990), Kohn & Little (1998) proved that if  $K_{\text{hom}}$  is invariant under rotation by  $\pi/2$ ,  $K_{\text{hom}}$  is contained in the ball of radius  $\sqrt{2M}$  centred at the origin. For polycrystals that are both isotropic and statistically isotropic, the Taylor bound is sharper than the Kohn–Little bound for values of  $M$  in a bounded interval. This is not surprising because the Taylor bound uses the information that every orientation occurs with equal probability and the Kohn–Little bound does not. Thus, the question arises of whether the translation method and the fact that the polycrystal is both isotropic and statistically isotropic can be combined to improve upon both bounds. Nesi *et al.* (2000) answer this question affirmatively. They derived two bounds. The sharpest one (which is valid under the assumption that the microgeometry of the polycrystal is isotropic) was obtained by combining ideas from the translation method with the technique developed by Talbot & Willis (1985). While this bound improves upon both the Taylor and the Kohn–Little bound, it seems to coincide with the latter for values of  $M$  larger than 3.5 (see Nesi *et al.* 2000). In §4 we derive a bound that improves upon all the above-mentioned bounds for large values of  $M$  ( $M \geq M_0$ , where  $M_0 < 2.5$ ). More precisely, we show that if the yield set of any polycrystal contains a ball of radius  $\rho$ , then  $\rho \leq 4\sqrt{M}/\pi$ . This result implies that the yield set of any isotropic polycrystal is contained in the ball of radius  $4\sqrt{M}/\pi$  centred at the origin.

Kohn & Little (1998) derived their bound by considering simultaneously two stress fields whose averages have perpendicular directions. However, it is known that for isotropic nonlinear materials, the translation method will deliver better bounds if we consider simultaneously not only two but several stress fields whose averages have different directions (see the comments by Milton & Serkov (2000)). Our analysis is based on this observation.

This same problem was also studied by Ponte Castañeda & Nebozhyn (1997) who obtained estimates of  $K_{\text{hom}}$  following the variational procedure of deBotton & Ponte Castañeda (1995). They also considered polycrystals whose grains' behaviour is described by power-law creep. Their results approximate  $K_{\text{hom}}$  by a ball that remains smaller than both the Taylor and the Kohn–Little bounds for all values of  $M$ . The variational technique of deBotton & Ponte Castañeda (1995) was also applied to estimates obtained for three-dimensional polycrystals (Nebozhyn *et al.* 2000, 2001; Gilormini *et al.* 2001).

## 2. Governing equations

The behaviour of a rigid perfectly plastic single crystal is characterized by a closed convex set  $K$  in the space of stresses (i.e. symmetric  $3 \times 3$  real matrices). The set  $K$  is related to the slip systems of the crystal (see, for example, Hirth & Lothe 1982; Lubliner 1990). This idealized material can only withstand stresses in  $K$ . If the material is subject to a stress  $\sigma$  which is in the interior of  $K$ , it does not deform. On the other hand, if  $\sigma \in \partial K$  (the boundary of  $K$ ), plastic flow occurs (i.e. the material will deform at a certain strain rate).  $K$  is called the yield set.

The texture of a polycrystal is determined by a rotation valued function  $R(x)$ . More precisely,  $R(x)$  denotes the orientation of the grain that contains the point  $x$ . If the yield set of the reference single crystal (i.e. its orientation is the identity matrix) is  $K$ , then the yield set of a single crystal whose orientation is  $R$  is  $RKR^T$ . Thus, a polycrystal can only withstand stresses  $\sigma$  that satisfy the pointwise constraint

$$R^T(x)\sigma(x)R(x) \in K \quad (2.1)$$

and the equilibrium equations

$$\nabla \cdot \sigma = 0. \quad (2.2)$$

Let  $\Omega$  be the region that the polycrystal occupies. Suppose that  $R(x)$  is periodic with period cell  $Q$ . In the limit in which the dimensions of  $Q$  are much smaller than those of  $\Omega$ , the polycrystal behaves as a rigid perfectly plastic material whose yield set is

$$K_{\text{hom}} = \{\tau : \tau = \langle \sigma \rangle, \text{ for some } Q\text{-periodic } \sigma \text{ satisfying (2.1) and (2.2)}\}. \quad (2.3)$$

In the above equation we have used the notation

$$\langle \sigma \rangle = \frac{1}{|Q|} \int_Q \sigma(x) dx. \quad (2.4)$$

See Bouchitté (1986), Bouchitté & Suquet (1991), de Buhan & Taliercio (1991), Demengel & Qi (1990), Jikov *et al.* (1994), Sab (1994) and Suquet (1987) for a mathematical justification of (2.3) as well as the analogous definition for random materials. (Note that the above statement is valid when the material is subjected to applied volume loads, but it might be false in the presence of applied surface loads. See the references mentioned for a detailed discussion.)

We will consider the above problem in the anti-plane shear context. More precisely, we assume that each grain occupies a region of the form  $G \times \mathbb{R}$ , where  $G \subseteq \mathbb{R}^2$  and that  $R(x)$  is a rotation that keeps the  $x_3$ -axis fixed (for all  $x$ ), and we restrict our attention to average stresses whose component  $\langle \sigma_{ij} \rangle$  may be different from 0 only if  $i \neq j$  and one of the indexes ( $i$  or  $j$ ) is equal to 3. Thus, due to symmetry, we also have that  $\sigma_{ij}(x)$  may be different from 0 only if  $i \neq j$  and one of the indexes is equal to 3. Under these conditions, the problem reduces to a two-dimensional one. More precisely, we rename the non-zero components of the stress as  $\sigma_i = \sigma_{i3}$  ( $i = 1, 2$ ) and we denote by  $\sigma$  the two-dimensional vector  $\sigma = (\sigma_1, \sigma_2)$ . The yield set of the reference single crystal is now a closed convex set in  $\mathbb{R}^2$ , which we also denote by  $K$ , and the condition (2.1) reduces to

$$R^T(x)\sigma(x) \in K, \quad (2.5)$$

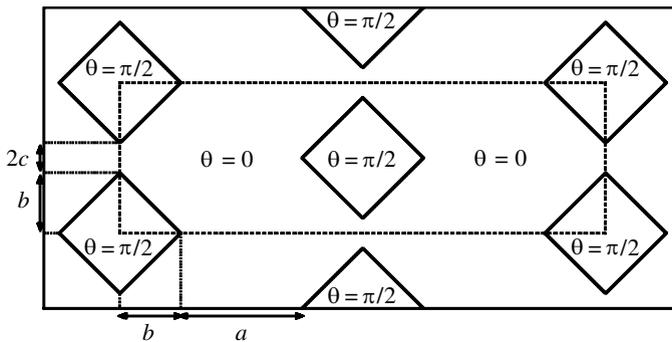


Figure 1. Texture of a polycrystal. The rectangle determined by the dashed lines is the period cell  $Q$ . The orientation inside the squares is  $\theta = \pi/2$ . The orientation outside the squares is  $\theta = 0$ . The values of the parameters that appear in this figure are  $a = \varepsilon$ ,  $b = \varepsilon/\sqrt{M}$  and  $c = \varepsilon/M$ .

where  $R(x)$  is now a  $2 \times 2$  rotation and  $x \in \mathbb{R}^2$ . Note that the rotation  $R(x)$  is determined by an angle  $\theta(x)$

$$R(x) = R_{\theta(x)} = \begin{bmatrix} \cos(\theta(x)) & -\sin(\theta(x)) \\ \sin(\theta(x)) & \cos(\theta(x)) \end{bmatrix}. \tag{2.6}$$

Following Kohn & Little (1998), we will assume that the yield set of the reference single crystal is

$$K = \{\sigma \in \mathbb{R}^2 : |\sigma_1| \leq M \text{ and } |\sigma_2| \leq 1\}, \tag{2.7}$$

where  $M \geq 1$ . As mentioned in § 1, Kohn & Little (1998) showed that, for statistically isotropic polycrystals, the Sachs and Taylor bounds predict the yield set of the polycrystal to be

$$\left. \begin{aligned} K_{\text{Sachs}} &= \{\tau \in \mathbb{R}^2 : \|\tau\| \leq 1\}, \\ K_{\text{Taylor}} &= \{\tau \in \mathbb{R}^2 : \|\tau\| \leq 2(M + 1)/\pi\}, \end{aligned} \right\} \tag{2.8}$$

respectively. In the above equations,  $\|\tau\| = \sqrt{\tau_1^2 + \tau_2^2}$  denotes the two-norm of  $\tau$ . Kohn & Little (1998) also proved that if  $K_{\text{hom}}$  is invariant under rotation by  $\pi/2$ , then

$$K_{\text{hom}} \subseteq K_{\text{KL}} = \{\tau \in \mathbb{R}^2 : \|\tau\| \leq \sqrt{2M}\}. \tag{2.9}$$

### 3. A family of polycrystals whose yield sets are large in all directions

Consider the polycrystal whose texture is described in figure 1. The values of the parameters that appear in figure 1 are  $a = \varepsilon$ ,  $b = \varepsilon/\sqrt{M}$  and  $c = \varepsilon/M$ . (Note that we have defined a family of polycrystals, one polycrystal for each value of  $M$ .) This choice of the parameters  $a$ ,  $b$  and  $c$  implies that the stress field  $\sigma$  displayed in figure 2 satisfies the equilibrium equation (2.2). The definition of  $\sigma$  is extended to  $\mathbb{R}^2$  by requiring that  $\sigma(x) = \sigma(x + v_1) = \sigma(x + v_2)$ , where  $v_1 = (0, 2(c + b))$  and  $v_2 = (2b + a, b + c)$ .

A simple calculation shows that the average of  $\sigma$  is  $\langle \sigma \rangle = \sqrt{M}(1, -1) + (O(1), O(1))$ . Since  $\sigma$  is an admissible stress field (i.e. equation (2.5) is satisfied for

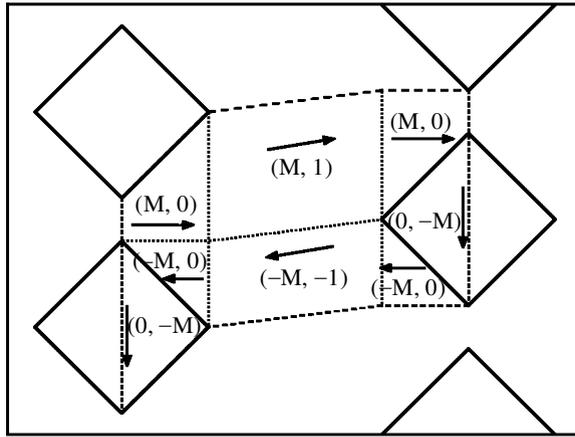


Figure 2. The stress field  $\sigma$ . The texture of this polycrystal is displayed in figure 1. The definition of  $\sigma$  is extended to  $\mathbb{R}^2$  by requiring that  $\sigma(x) = \sigma(x + v_1) = \sigma(x + v_2)$ , where  $v_1 = (0, 2(c + b))$  and  $v_2 = (2b + a, b + c)$  (see figure 1).

all  $x$ ) and given the symmetry of the texture of the polycrystal under consideration and the convexity of  $K_{\text{hom}}$ , we conclude that the effective yield set of the polycrystal in question contains a square of the form  $[-f, f]^2$ , where  $f = \sqrt{M} - O(1)$ .

As  $M$  becomes large, this polycrystal behaves as a very hard material in every direction. On the other hand, Kohn & Little (1998) showed an example of a polycrystal that is ductile in every direction (i.e. with yield set bounded) independent of the value of  $M$ . Thus, for large values of  $M$  (highly anisotropic grains), polycrystals with different texture may exhibit extremely different behaviour.

#### 4. Improved bounds on the yield set of isotropic polycrystals

##### (a) The Kohn–Little bound

The Kohn–Little bound is based on the fact that

$$\det[\tau^{(1)}, \tau^{(2)}] = \langle \det[\sigma^{(1)}, \sigma^{(2)}] \rangle, \quad \text{where } \tau^{(i)} = \langle \sigma^{(i)} \rangle \tag{4.1}$$

for any pair of divergence-free fields of stresses  $\sigma^{(1)}$  and  $\sigma^{(2)}$  (see Kohn & Little 1998). (In the above equation,  $[\tau^{(1)}, \tau^{(2)}]$  denotes the matrix whose  $i$ th column is  $\tau^{(i)}$ , and, similarly,  $[\sigma^{(1)}, \sigma^{(2)}]$  is the matrix whose  $i$ th column is  $\sigma^{(i)}$ .)

More precisely, the derivation of the Kohn–Little bound is as follows. Let  $\tau^{(2)} = R_{\pi/2}\tau^{(1)}$  ( $R_{\pi/2}$  is the rotation by  $\pi/2$ ; see (2.6)). We thus have that the left-hand side of the first equation in (4.1) is  $\|\tau^{(1)}\|^2$ . Assume that both  $\tau^{(1)}$  and  $\tau^{(2)}$  belong to  $K_{\text{hom}}$  and let  $\sigma^{(1)}$  and  $\sigma^{(2)}$  be admissible stress fields associated with  $\tau^{(1)}$  and  $\tau^{(2)}$ , respectively (i.e.  $\sigma^{(i)}$  satisfies (2.2) and (2.5), and  $\tau^{(i)} = \langle \sigma^{(i)} \rangle$  for both  $i = 1$  and  $i = 2$ ). The pointwise restriction (2.5) implies that  $\det[\sigma^{(1)}, \sigma^{(2)}] \leq 2M$  for all  $x$ , and as a consequence the right-hand side of the first equation in (4.1) is bounded by  $2M$ . It is thus concluded that if both  $\tau$  and  $R_{\pi/2}\tau$  belong to  $K_{\text{hom}}$ , then  $\|\tau\|^2 \leq 2M$ . In particular, if the polycrystal is isotropic, the Kohn–Little bound implies that  $K_{\text{hom}}$  is included in the ball of radius  $\sqrt{2M}$  centred at the origin.

## (b) Improved bounds

It is known that for isotropic nonlinear materials, the translation method will deliver better bounds if we consider simultaneously not only two but several stress fields whose averages have different directions (see the comments by Milton & Serkov (2000)). We now follow this observation to derive a new bound on the yield set of isotropic polycrystals.

Consider a family of divergence-free stress fields  $\sigma$ , parametrized by the angle  $\phi$ ,  $\sigma = \sigma_\phi = \sigma_\phi(x)$ , with the property that

$$\langle \sigma_\phi \rangle = \rho(\cos(\phi), \sin(\phi)) \quad (4.2)$$

for some  $\rho \geq 0$ . For convenience, assume this family to be  $2\pi$ -periodic (i.e.  $\sigma_{\phi+2\pi}(x) = \sigma_\phi(x)$  for all  $x$ ). Equation (4.1) implies that

$$\rho^2 \sin(\beta) = \langle \det[\sigma_\phi, \sigma_{\phi+\beta}] \rangle \quad \text{for all } \phi \text{ and } \beta. \quad (4.3)$$

Let  $\mathcal{F}$  be the set of functions of two variables,  $f = f(\beta, \phi)$ , that are  $2\pi$ -periodic in both variables and satisfy

$$\int_0^{2\pi} \int_0^{2\pi} f(\beta, \phi) \sin(\beta) \, d\beta \, d\phi = 1. \quad (4.4)$$

For any  $f \in \mathcal{F}$ , equations (4.3) and (4.4) clearly imply that

$$\rho^2 = \int_0^{2\pi} \int_0^{2\pi} f(\beta, \phi) \langle \det[\sigma_\phi, \sigma_{\phi+\beta}] \rangle \, d\beta \, d\phi. \quad (4.5)$$

After defining

$$G(x) = \int_0^{2\pi} \int_0^{2\pi} f(\beta, \phi) \det[\sigma_\phi(x), \sigma_{\phi+\beta}(x)] \, d\beta \, d\phi \quad (4.6)$$

and changing the order of integration in (4.5), we have

$$\rho^2 = \langle G \rangle. \quad (4.7)$$

Since the determinant of any rotation matrix is 1,  $G(x)$  can be written as

$$G(x) = \int_0^{2\pi} \int_0^{2\pi} f(\beta, \phi) \det[R^T(x)\sigma_\phi(x), R^T(x)\sigma_{\phi+\beta}(x)] \, d\beta \, d\phi. \quad (4.8)$$

We denote by  $\mathcal{Y}$  the set of  $2\pi$ -periodic functions of one variable that are pointwise bounded by 1 in absolute value

$$\mathcal{Y} = \{y : y \text{ is } 2\pi\text{-periodic and } |y(\phi)| \leq 1 \text{ for all } \phi\}. \quad (4.9)$$

Assuming that  $\sigma_\phi$  satisfies (2.5) for all  $\phi$  and all  $x \in Q$ , equations (2.7) and (4.8) imply that

$$G(x) \leq M \sup_{y, z \in \mathcal{Y}} \int_0^{2\pi} \int_0^{2\pi} f(\beta, \phi) \det \begin{bmatrix} y(\phi) & y(\phi + \beta) \\ z(\phi) & z(\phi + \beta) \end{bmatrix} \, d\beta \, d\phi. \quad (4.10)$$

Equations (4.6), (4.7) and (4.10) are valid for all  $f \in \mathcal{F}$ ; thus, taking the infimum over all  $f \in \mathcal{F}$ , we obtain that

$$\rho \leq \rho_* \sqrt{M}, \quad (4.11)$$

where  $\rho_*$  is the positive number defined by

$$\rho_*^2 = \inf_{f \in \mathcal{F}} \sup_{y, z \in \mathcal{Y}} \int_0^{2\pi} \int_0^{2\pi} f(\beta, \phi) \det \begin{bmatrix} y(\phi) & y(\phi + \beta) \\ z(\phi) & z(\phi + \beta) \end{bmatrix} d\beta d\phi. \quad (4.12)$$

We conclude that if the ball of radius  $\rho$  (centred at the origin) is included in  $K_{\text{hom}}$ , then  $\rho \leq \rho_* \sqrt{M}$ . In particular, if the polycrystal is isotropic, we have

$$K_{\text{hom}} \subseteq \{\tau \in \mathbb{R}^2 : \|\tau\| \leq \rho_* \sqrt{M}\}. \quad (4.13)$$

The exact solution of (4.12) has proven to be difficult. Nevertheless, the evaluation of the right-hand side of (4.10) for any  $f \in \mathcal{F}$  will produce an upper bound. In particular, we show in Appendix A that the choice  $f(\beta, \phi) = \sin(\beta)/(2\pi^2)$  gives us  $\rho_* \leq 4/\pi$  and thus,

$$K_{\text{hom}} \subseteq \left\{ \tau \in \mathbb{R}^2 : \|\tau\| \leq \frac{4}{\pi} \sqrt{M} \right\} \quad (4.14)$$

if the polycrystal is isotropic. Note that this bound is sharper than both the Taylor and the Kohn–Little bounds for any value of  $M$ .

## 5. Conclusions

We have restricted our attention to the anti-plane shear context.

We have constructed polycrystals that are very hard in every direction even though their grains have one ductile direction (the orthogonal direction being rigid). On the other hand, there are polycrystals (whose grains have one ductile and one rigid direction) that are ductile in every direction (see Kohn & Little 1998). Thus, if the grains are highly anisotropic, polycrystals with different textures may exhibit extremely different behaviour.

We have also derived an outer bound on the yield set of isotropic polycrystals. More precisely, we have shown that the yield set of any isotropic polycrystal is contained in the ball of radius  $4\sqrt{M}/\pi$  centred at the origin. This outer bound can be regarded as a generalization of the analysis by Kohn & Little (1998). More precisely, the Kohn–Little bound results from considering simultaneously two stress fields whose averages have perpendicular directions. To obtain the bound presented in this paper, we have considered not only two but several stress fields whose averages have different directions.

The class of rigid perfectly plastic polycrystals studied in this paper has proven to be amenable to mathematical analysis. Given the results of this work, the natural next step is to incorporate more information about the texture in the analysis. It is also desirable to consider three-dimensional polycrystals. In this regard, the variational technique of deBotton & Ponte Castañeda (1995) was used to study three-dimensional polycrystals (Nebozhyn *et al.* 2000, 2001; Gilormini *et al.* 2001).

I thank Professor Kohn for making me aware of the work (Kohn & Little 1998) that motivated the present study. I also thank the reviewers for their suggestions.

## Appendix A.

We now proceed with the evaluation of the bound (4.14). More precisely, we have to show that

$$\frac{16}{\pi^2} = \frac{1}{2\pi^2} \max_{y,z \in \mathcal{Y}} \int_0^{2\pi} \int_0^{2\pi} \sin(\beta) \det \begin{bmatrix} y(\phi) & y(\phi + \beta) \\ z(\phi) & z(\phi + \beta) \end{bmatrix} d\beta d\phi, \quad (\text{A } 1)$$

where  $\mathcal{Y}$  was defined in (4.9).

The first step is to note that

$$4 \operatorname{Im}(\hat{y}_1 \hat{z}_{-1}) = \frac{1}{2\pi^2} \int_0^{2\pi} \int_0^{2\pi} \sin(\beta) \det \begin{bmatrix} y(\phi) & y(\phi + \beta) \\ z(\phi) & z(\phi + \beta) \end{bmatrix} d\beta d\phi, \quad (\text{A } 2)$$

where

$$\hat{y}_1 = \frac{1}{2\pi} \int_0^{2\pi} y(\phi) e^{-i\phi} d\phi, \quad \hat{z}_{-1} = \frac{1}{2\pi} \int_0^{2\pi} z(\phi) e^{i\phi} d\phi, \quad (\text{A } 3)$$

and  $\operatorname{Im}(\hat{y}_1 \hat{z}_{-1})$  denotes the imaginary part of  $\hat{y}_1 \hat{z}_{-1}$ .

Next, from simple arguments it can be shown that

$$\max_{y,z \in \mathcal{Y}} \operatorname{Im}(\hat{y}_1 \hat{z}_{-1}) = \max_{y \in \mathcal{Y}} |\hat{y}_1|^2. \quad (\text{A } 4)$$

Finally, we observe that the maximum in (A 4) is attained at the function  $y(\phi) = \operatorname{sgn}(\sin(\phi))$  ( $y(\phi) = 1$  if  $\sin(\phi) \geq 0$  and  $y(\phi) = -1$  if  $\sin(\phi) < 0$ ) and thus, a simple calculation, equations (A 4) and (A 2) confirm the validity of (A 1).

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