Some three-dimensional problems related to dielectric breakdown and polycrystal plasticity

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Abstract

The well-known Sachs and Taylor bounds provide easy inner and outer estimates for the effective yield set of a polycrystal. It is natural to ask whether they can be improved. We examine this question for two model problems, involving 3D gradients and divergence-free vector fields. For 3D gradients the Taylor bound is far from optimal: we derive an improved estimate which scales differently when the yield set of the basic crystal is highly eccentric. For 3D divergence-free vector fields the Taylor bound may not be optimal, but it has the optimal scaling law. In both settings the Sachs bound is optimal.

1 Introduction

The analysis of rigid, perfectly-plastic polycrystals leads to an interesting class of homogenization problems with L^∞ constraints. A polycrystal is described in this context by the shapes and orientations of its grains, and the yield set $K_{\rm bas}$ of its basic crystal. The homogenization problem determines from these ingredients an effective yield set $K_{\rm eff}$. There are relatively simple inner and outer estimates, known as the Sachs and Taylor bounds, such that

$$K_{\rm Sachs} \subset K_{\rm eff} \subset K_{\rm Taylor}.$$

It is natural to ask whether these bounds are optimal – and if not then to seek improved estimates of $K_{\rm eff}$.

A fresh approach to this class of problems was suggested in [9]. It (i) focuses on cases when $K_{\rm bas}$ is highly eccentric, and (ii) considers model problems involving gradients or divergence-free vector fields. Both reductions are physically natural: crystals with few slip systems are described by eccentric or unbounded yield sets $K_{\rm bas}$; and dielectric breakdown is described by an L^∞ homogenization problem involving gradient fields.

The reduction (i) is convenient because when $K_{\rm bas}$ is large in some direction, $K_{\rm Taylor}$ is large in all directions. Thus, rather than ask whether $K_{\rm Taylor}$ is optimal, we can ask the more qualitative question whether it achieves the optimal scaling law.

The reduction (ii) is necessary because the direct analysis of 3D plasticity problems (involving divergence-free stress tensors) is presently out of reach. By considering simpler model problems, we gain intuition and develop appropriate methods. We also gain valuable benchmarks, which can be to assess the adequacy of various self-consistent schemes [14].

Recent papers pursuing this approach include [7, 8, 9, 12, 17]. Most of this work addresses model problems involving 2D divergence-free vector fields. Kohn and Little [9] showed that the Sachs bound is optimal in this 2D setting but the Taylor bound is not, and they gave a new outer estimate with a better scaling law. Their result was improved by Goldsztein [7], who gave an outer bound with the same scaling law but a better constant. Goldsztein has also shown that this scaling law is essentially optimal [8]. Since 2D divergence-free vector fields can be represented as curls, these results apply equally to model problems involving 2D gradient fields.

This paper considers analogous 3D problems involving gradients and divergence-free vector fields. For 3D gradients, we show that the Sachs bound is optimal but the Taylor bound can be improved. Moreover we explore two different schemes for improving on the Taylor bound: one using a linear comparison material, the other using the 3D determinant as a null-Lagrangian. The latter gives a better scaling law. This is different from the situation in 2D, where both schemes give the same (essentially optimal) scaling law.

For 3D divergence-free vector fields, we show that the Sachs bound is again optimal. Moreover we show that the Taylor bound, though possibly not optimal, has the optimal scaling law. Thus the status of the Taylor bound is quite different for 3D divergence-free vector fields from the other cases considered to date.

Detailed introductions to this subject can be found in [6, 7, 9]. Therefore we shall be relatively brief, providing only the background required to establish our notation and present our results.

In plasticity the Sachs and Taylor bounds are associated with constant-stress and constant-strain test fields respectively. Our convention is consistent with this but slightly different: the Sachs bound is the natural *inner* estimate, and the Taylor bound the natural *outer* estimate (this is different from the convention of [3]).

2 3D gradient fields

The problem considered in this section can be viewed as a warmup toward polycrystal plasticity. Or, as explained e.g. in [6], it can be viewed as a model of (first failure) dielectric breakdown of a 3D polycrystalline insulator.

For the basic crystal, we suppose the potential $\phi : \mathbf{R}^3 \to \mathbf{R}$ satisfies the pointwise constraint

$$\nabla\phi(x) \in K_{\mathrm{bas}} \quad \text{for a.e. } x.$$

Here K_{bas} is a convex set – the yield set of the basic crystal. We shall consider K_{bas} of the form

$$K_{M,N} = \{\xi \in \mathbf{R}^3 \,:\, |\xi_1| \leq 1,\ |\xi_2| \leq M,\ |\xi_3| \leq N\} \tag{2.1}$$

with $1 \leq M \leq N$.

We consider spatially periodic polycrystals made from this basic crystal. There is no loss of generality in taking the period cell Q to be the unit cube:

$$Q = [0,1]^3 \subset \mathbf{R}^3.$$

The polycrystalline texture is determined by a rotation field $R(x)$, giving the orientation of the basic crystal at $x \in Q$. The effective behavior is determined by considering potentials ϕ satisfying the pointwise constraint

$$\nabla\phi(x) \in R(x)K_{M,N} \quad \text{for a.e. } x \tag{2.2}$$

and such that $\nabla\phi$ is Q-periodic. The effective yield set K_{eff} is the set of all mean values

$$\xi = \int_Q \nabla\phi(x)\,dx$$

consistent with (2.2). Since

$$\nabla\phi \text{ is periodic with mean value } \xi \iff \phi = \xi\cdot x + u(x) \text{ with } u \text{ periodic,}$$

we have

$$\begin{aligned} K_{\text{eff}} &= \{\xi\in\mathbf{R}^3 \ :\ \text{there exists a } Q\text{-periodic, } W^{1,\infty} \\ &\qquad\qquad \text{function } u \text{ with } \nabla u + \xi \in R(x)K_{M,N} \text{ a.e.}\} \end{aligned} \tag{2.3}$$

The Sachs bound is obtained by restricting attention to constant $\nabla\phi$. This amounts to taking $u=0$; it gives

$$K_{\text{Sachs}} = \text{ the set of all vectors } \xi \text{ satisfying } \xi\in R(x)K_{M,N} \text{ for a.e. } x. \tag{2.4}$$

The Taylor bound is obtained by replacing the curl-free vector field ∇u by an arbitrary periodic one; this gives

$$K_{\text{Taylor}} = \text{ the set of all averages } \textstyle\int_Q g\,dx \text{ where } g(x)\in R(x)K_{M,N} \text{ for a.e. } x. \tag{2.5}$$

It is obvious from the definitions that

$$K_{\text{Sachs}} \subset K_{\text{eff}} \subset K_{\text{Taylor}}.$$

These bounds are easy to evaluate. Clearly

$$K_{\text{Sachs}} = \cap_x R(x)K_{M,N},$$

so the Sachs bound depends only on the list of rotations present in the polycrystal. If every rotation occurs then clearly

$$K_{\text{Sachs}} \text{ is the ball of radius 1.} \tag{2.6}$$

The Taylor bound depends on more than just the list of rotations present – it incorporates the one-point statistics of the polycrystal, i.e. the local proportions of the rotations present in it. If every rotation occurs with equal probability then

$$K_{\text{Taylor}} \text{ is the ball of radius } (1+M+N)/2. \tag{2.7}$$

Indeed, for any $\eta\in\mathbf{R}^3$ we have

$$\begin{aligned} \max_{\xi\in K_{\text{Taylor}}} \xi\cdot\eta &= \int_Q \max_{g(x)\in R(x)K_{M,N}} g\cdot\eta\,dx \\ &= \int_Q |R^T(x)\eta\cdot e_1| + M|R^T(x)\eta\cdot e_2| + N|R^T(x)\eta\cdot e_3|\,dx. \end{aligned}$$

If the rotations are equidistributed then the vectors $R^T(x)e_i$ are uniformly distributed on the sphere for each i. It follows that

$$\int_Q |R^T(x)\eta\cdot e_i|\,dx = |\eta|\int_{S^2}|\xi\cdot e_i|\,d\xi = \frac{1}{2}|\eta|.$$

Thus

$$\max_{\xi\in K_{\text{Taylor}}} \xi\cdot\eta = \frac{1+M+N}{2}|\eta|,$$

which implies (2.7).

2.1 An improved outer bound using the 3D determinant

The Taylor bound grows linearly as $N \to \infty$. However a better bound – with a better scaling law – is possible. The following result and its proof are analogous to Proposition 5.3 of [9].

Proposition 1 *If three vectors ξ, η, and ζ are all in K_{eff} then*

$$det\,(\xi, \eta, \zeta) \leq 4MN\,. \tag{2.8}$$

In particular, if (for example due to symmetry) K_{eff} is a ball, then

$$\text{radius}\,(K_{\text{eff}}) \leq (4MN)^{1/3}\,. \tag{2.9}$$

Proof. We begin by observing that

$$\max_{\xi,\eta,\zeta \in K_{M,N}} \det\,(\xi, \eta, \zeta) = 4MN\,. \tag{2.10}$$

Indeed, the choice $\xi = (1, M, N)$, $\eta = (1, M, -N)$, $\zeta = (-1, M, N)$ shows that the max is at least $4MN$. Since the determinant is multilinear and $K_{M,N}$ is a convex polygon, it suffices to consider ξ, η, ζ which are vertices. One verifies, e.g. by enumerating all possibilities, that the value $4MN$ is maximal.

Now suppose ξ, η, ζ belong to K_{eff}. Then, by definition, there exist three functions ϕ, ψ and χ, with $\nabla\phi$, $\nabla\psi$, and $\nabla\chi$ periodic, such that

$$\xi = \int_Q \nabla\phi(x)\,dx\,, \qquad \eta = \int_Q \nabla\psi(x)\,dx\,, \qquad \zeta = \int_Q \nabla\chi(x)\,dx\,,$$

and such that $\nabla\phi(x)$, $\nabla\psi(x)$, and $\nabla\chi(x)$ all lie in $R(x)K_{M,N}$ for a.e. x. Since the determinant is a rotationally-invariant null-lagrangian, we conclude that

$$\begin{aligned} \det\,(\xi, \eta, \zeta) &= \int_Q \det\,(\nabla\phi(x), \nabla\psi(x), \nabla\chi(x))\,dx\,, \\ &\leq \int_Q 4MN\,dx = 4MN\,. \end{aligned}$$

This establishes (2.8); if K_{eff} is isotropic then (2.9) follows by choosing ξ, η, and ζ to be mutually orthogonal. ○

The preceding bound is probably not optimal. The analogous 2D result was improved upon slightly by using the full force of the translation method [12, 17]. Much greater improvement was obtained, for isotropic polycrystals, by using a continuum of test fields [7]. We suppose similar improvements are possible in the present 3D setting. We doubt, however, that they would change the associated scaling law for isotropic polycrystals: $\text{radius}\,(K_{\text{eff}}) \leq C(MN)^{1/3}$ for $1 \leq M \leq N \to \infty$. It remains an open question whether this scaling law is optimal; the analogous 2D question was settled affirmatively in [8].

2.2 A weaker outer bound using the linear comparison method

The linear comparison method is a scheme – really a family of schemes – for bounding nonlinear effective behavior by combining (a) information about the effective behavior of related linear composites, with (b) microstructure-independent algebraic arguments. This approach is flexible because we know quite a bit about linear composites. It is moreover rather general: unlike the method of Section 2.1, the linear comparison technique is not limited to our model problems — it extends naturally to physically realistic settings [11, 13, 14].

By studying model problems, we gain insight concerning the intrinsic power of the linear comparison method. The analysis of [9] suggests optimism: in the 2D scalar setting considered there, for polycrystals with sufficient symmetry, linear comparison gives the same (essentially optimal) scaling law as the null-Lagrangian method.

The results in this section suggest caution. Indeed, in our 3D scalar setting (and for our particular implementation) linear comparison gives a scaling law inferior to that of the null-Lagrangian method.

We are not sure what lesson to draw from this result. Perhaps our implementation of the linear comparison method is suboptimal. Or maybe there is an essential difference in 3D between the null-Lagrangian and linear comparison techniques, arising from their different homogeneities – since the 3D determinant is cubic while the energy of a linear comparison material is quadratic.

Speculating further: our L^∞-constrained homogenization problems have a sort of percolation character – see e.g. the constructions in [7, 8, 9] (and, in a slightly different setting, [3, 4]). So perhaps the problem of bounding K_{eff} is related to the linking of curves, hence to topological degree and the 3D determinant. Or maybe not: the analysis of linear polycrystals with highly eccentric Hooke's laws has a similar percolation character [5], yet optimal bounds have been proved in that setting using only quadratic null-Lagrangians [2].

Our linear comparison bound is directly analogous to Proposition 6.1 of [9]. However our proof uses the strategy of [6], which is much simpler than that of [9].

The heart of the matter is an optimal lower bound proved in [2, 15, 16] for the effective conductivity of a 3D linear polycrystal. We briefly review this result. For any $\sigma_1, \sigma_2, \sigma_3 > 0$ and any rotation field $R(x)$, consider the linear polycrystal whose local conductivity tensor is

$$R(x) \begin{pmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{pmatrix} R^T(x).$$

Let σ_* be its effective conductivity. Then we have the bound

$$\frac{1}{3} \mathrm{Tr}\, \sigma_* \geq \sigma_s \tag{2.11}$$

where σ_s is the unique positive root of

$$\sigma_s^3 + (\sigma_1 + \sigma_2 + \sigma_3)\sigma_s^2 - 4\sigma_1\sigma_2\sigma_3 = 0. \tag{2.12}$$

We shall apply (2.11) with the specific choice

$$\begin{gathered} \sigma_1 = 1, \quad \sigma_2 = 1/M^2, \quad \sigma_3 = 1/N^2, \\ R(x) = \text{orientation of the nonlinear polycrystal, as in (2.2.)} \end{gathered} \tag{2.13}$$

Proposition 2 *Suppose (for example due to symmetry) the linear comparison crystal (2.13) is isotropic, in the sense that its effective conductivity $\sigma_*(M,N)$ is a multiple of the identity. Then every $\xi \in K_{\mathrm{eff}}$ satisfies*

$$|\xi| \leq \left(\frac{3}{\sigma_s(M,N)} \right)^{1/2} \tag{2.14}$$

where $\sigma_s(M,N)$ is defined by (2.12) with σ_i determined by (2.13). Moreover

$$\sigma_s(M,N) \geq \frac{2}{\sqrt{5}MN}. \tag{2.15}$$

Thus if K_{eff} is isotropic the bound becomes

$$\mathrm{radius}\,(K_{\mathrm{eff}}) \leq (\tfrac{3\sqrt{5}}{2} MN)^{1/2}\,. \tag{2.16}$$

Notice that (2.16) is weaker than (2.9), since $(MN)^{1/2} \gg (MN)^{1/3}$ when $MN \gg 1$.

Proof. If $\xi \in K_{\rm eff}$, then there exists a periodic, $W^{1,\infty}$ function u satisfying $\xi + \nabla u \in R(x)K_{M,N}$ a.e., i.e. such that

$$|\langle \nabla u + \xi, R(x)e_1\rangle| \le 1, \quad |\langle \nabla u + \xi, R(x)e_2\rangle| \le M, \quad |\langle \nabla u + \xi, R(x)e_3\rangle| \le N\,.$$

It follows that

$$\int_Q |\langle \nabla u + \xi, R(x)e_1\rangle|^2 + \frac{|\langle \nabla u + \xi, R(x)e_2\rangle|^2}{M^2} + \frac{|\langle \nabla u + \xi, R(x)e_3\rangle|^2}{N^2}\,dx \le 3.$$

Taking u as a test field in the definition of the effective conductivity tensor, this shows that our linear comparison polycrystal (2.13) has

$$\langle \sigma_* \xi, \xi\rangle \le 3.$$

Now we use the hypothesis that σ_* is isotropic, along with optimal lower bound (2.11). These give

$$\sigma_s(M,N)|\xi|^2 \le \frac{1}{3}{\rm Tr}\,(\sigma_*)|\xi|^2 = \langle \sigma_*\xi, \xi\rangle \le 3\,,$$

which yields (2.14). For (2.15), we observe first that $\sigma_s(M,N) \le 2/MN \le 2$; indeed, using the definition (2.12) of σ_s we have

$$\sigma_s^2(M,N) \le \sigma_s^3(M,N) + \left(1 + \frac{1}{N^2} + \frac{1}{M^2}\right)\sigma_s^2(M,N) = \frac{4}{N^2M^2}\,.$$

This upper bound leads easily to the lower bound (2.15):

$$5\sigma_s^2 \ge \left(1 + \frac{1}{N^2} + \frac{1}{M^2}\right)\sigma_s^2 + \sigma_s^3 = (\sigma_1 + \sigma_2 + \sigma_3)\sigma_s^2 + \sigma_s^3 = 4\sigma_1\sigma_2\sigma_3 = \frac{4}{M^2N^2}$$

using the hypothesis $M, N \ge 1$ in the first step. The final assertion (2.16) is an immediate consequence of (2.14) and (2.15). ○

2.3 The Sachs bound is optimal

We have shown that the Taylor bound is far from optimal, in the sense that a better bound – with a better scaling law – is possible. The situation is different for the Sachs bound. We show in this section that it is optimal, in the sense that there exist polycrystals with $K_{\rm eff} = K_{\rm Sachs}$.

A similar result holds in 2D (see Examples 1 and 2 of [9]). Actually examples are easier to construct in 3D because lines in different directions are generically disjoint. Our main tool is the following:

Lemma 3 *Consider a periodic polycrystal with orientation $R(x)$ and basic yield set $K_{M,N}$. Suppose there is a closed path γ on the torus with average tangent $\bar{t}$ such that*

- *γ stays a.e. in the set where $R(x)$ is smooth, and*
- *γ is tangent a.e. to $R(x)e_1$.*

Then every $\xi \in K_{\rm eff}$ satisfies $|\xi \cdot \bar{t}| \le 1$.

Proof. This is essentially Lemma 4.2 of [9]; we repeat the easy argument for the reader's convenience. If $\xi \in K_{\rm eff}$ then there is a periodic u satisfying $\xi + \nabla u \in R(x)K_{M,N}$ a.e.; in particular

$$|\langle \xi + \nabla u, R(x)e_1\rangle| \le 1 \quad \text{a.e. along } \gamma.$$

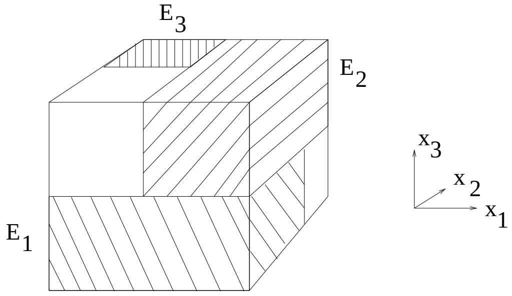

Figure 1: The sets E_1, E_2, and E_3.

Denoting by $t(s)$ the unit tangent vector along the path, we have

$$|\langle \xi + \nabla u, t(s)\rangle| \leq 1 \qquad \text{for a.e. } s$$

since $t(s) \| R(x)e_1$. Let L be the length of the path. We have

$$|\langle \xi, L\bar{t}\rangle| = \left| \int_{\text{path}} \langle \xi + \nabla u, t(s)\rangle \, ds \right|$$

since u is periodic and the path is closed (here ds is arclength). The right hand side is bounded by

$$\int_{\text{path}} |\langle \xi + \nabla u, t(s)\rangle| \, ds \leq L.$$

Division by L gives the desired result. ○

Example 1. Define regions $E_i \subset Q$ by

$$E_1 = (0,1) \times (0, \tfrac{1}{2})^2, \quad E_2 = (\tfrac{1}{2}, 1) \times (0,1) \times (\tfrac{1}{2}, 1), \quad E_3 = (0, \tfrac{1}{2}) \times (\tfrac{1}{2}, 1) \times (0,1)$$

(see Figure 1). Notice that these sets are disjoint, and E_i is a square cylinder with axis parallel to the coordinate direction e_i. Define rotations R_i by

$$R_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad R_2 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad R_3 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

and consider a polycrystal using just these rotations with

$$R(x) = R_1 \text{ on } E_1, \quad R(x) = R_2 \text{ on } E_2, \quad R(x) = R_3 \text{ on } E_3.$$

The value of $R(x)$ on $Q - (E_1 \cup E_2 \cup E_3)$ doesn't affect the argument – it can be chosen arbitrarily. Since $R_i e_1 = e_i$, we can apply Lemma 3 three times, choosing the path γ to be the axis of E_i, $i = 1, 2, 3$. It follows that the effective yield set of this polycrystal satisfies

$$\xi \in K_{\text{eff}} \Longrightarrow |\xi_i| \leq 1 \text{ for } i = 1, 2, 3.$$

But for a polycrystal using the three rotations R_i the Sachs bound is

$$K_{\text{Sachs}} = \cap_{i=1}^{3} R_i K_{M,N} = \{\xi \,:\, |\xi_i| \leq 1\}.$$

Thus $K_{\text{eff}} = K_{\text{Sachs}}$ as desired. ○

There is clearly a lot of freedom in this construction. All we really used in evaluating K_{eff} was the restriction of $R(x)$ to the three cylinder axes.

In our example $K_{\text{eff}} = K_{\text{Sachs}}$ is a cube. However a similar technique can be used to give examples where $K_{\text{eff}} = K_{\text{Sachs}}$ is a ball. For this purpose one must use infinitely many cylinders rather than just three; the argument is parallel to Theorem 3.8 of [6].

3 3D divergence-free fields

In Section 2 the basic fields were gradients. Here we consider the analogous problem with divergence-free vector fields instead of gradients.

The definition of K_{eff} is obvious. Our basic variables are now Q-periodic divergence free vector fields $\sigma(x)$, constrained by the analogue of (2.2):

$$\sigma(x) \in R(x) K_{M,N}\,. \tag{3.1}$$

Here $K_{M,N}$ is still defined by (2.1), and $R(x)$ is still a rotation-valued function giving the texture of the polycrystal. We define K_{eff} to be the set of all mean values

$$\xi = \int_Q \sigma(x)\,dx$$

consistent with (3.1). Thus the analogue of (2.3) is

$$\begin{aligned} K_{\text{eff}} \quad = \quad \{\xi \in \mathbf{R}^3 \ :\ & \text{there exists a } Q\text{-periodic, divergence-free vector field } \sigma(x) \\ & \text{with mean value } \xi \text{ such that } \sigma(x) \in R(x)K_{M,N} \text{ a.e.}\} \end{aligned} \tag{3.2}$$

The Sachs and Taylor bounds K_{Sachs} and K_{Taylor} are still given by (2.4) and (2.5), and exactly as before we have

$$K_{\text{Sachs}} \subset K_{\text{eff}} \subset K_{\text{Taylor}}\,.$$

3.1 The Taylor bound has the optimal scaling law

The Taylor bound scales linearly in N. For 3D gradients this is far from optimal – we gave a better bound (with a better scaling law) in Section 2.1. The situation is different, however, for divergence-free vector fields. Perhaps the Taylor bound can be improved, but no better scaling law is possible. To show this, we give an example of a polycrystal whose K_{eff} contains a ball of radius $N/4$.

Example 2. Let E_i and R_i be as in Example 1. This time however we take

$$R(x) = R_2 \text{ on } E_1, \quad R(x) = R_3 \text{ on } E_2, \quad R(x) = R_1 \text{ on } E_3.$$

As in Example 1, the value of $R(x)$ on $Q - (E_1 \cup E_2 \cup E_3)$ doesn't affect the argument; it can be chosen arbitrarily. We assert that for any such polycrystal

$$K_{\text{eff}} \text{ contains } \{\xi \ :\ |\xi|_\infty \le \tfrac{N}{4}\},$$

with the notation $|\xi|_\infty = \max_{i=1}^3 |\xi_i|$. To see this, for any ξ such that $|\xi|_\infty \le N/4$, we consider

$$\sigma(x) = \begin{cases} 4\xi_i e_i & \text{for } x \in E_i,\ i = 1,2,3 \\ 0 & \text{otherwise.} \end{cases}$$

Clearly σ is divergence-free, and its average value is ξ. The admissibility condition (3.1) boils down to

$$4\xi_1 e_1 \in R_2 K_{M,N}, \quad 4\xi_2 e_2 \in R_3 K_{M,N}, \quad \text{and} \quad 4\xi_3 e_3 \in R_1 K_{M,N}. \tag{3.3}$$

But $K_{M,N}$ is long in direction 3, and

$$R_2 e_3 = e_1, \quad R_3 e_3 = e_2, \quad \text{and} \quad R_1 e_3 = e_3,$$

so (3.3) is satisfied when $4|\xi|_\infty \le N$. ○

3.2 The Sachs bound is optimal

The Sachs bound is independent of M and N. Section 2.3 showed it was optimal for 3D gradients. This section shows it is also optimal for divergence-free vector fields.

We shall use the following elementary result.

Lemma 4 *If σ is a Q-periodic, L^∞, divergence-free vector field, then for $i = 1, 2, 3$ the average of $\sigma \cdot e_i$ on the hyperplane $x_i = t$ is independent of t.*

Proof. Recall that an L^∞ divergence-free vector field has a well-defined normal trace $\sigma \cdot \nu$ on any Lipschitz hypersurface Γ, see e.g. [1, 10, 18]. Thus $\sigma \cdot e_i$ is well-defined on each hyperplane $x_i = t$. To show it is independent of t, we apply Green's formula on the region $Q \cap \{t < x_i < t'\}$:

$$\int_{Q\cap\{x_i=t'\}} \sigma \cdot e_i \, dx - \int_{Q\cap\{x_i=t\}} \sigma \cdot e_i \, dx = \int_{Q\cap\{t<x_i<t'\}} \operatorname{div} \sigma \, dx = 0$$

(the remaining boundary terms cancel, by periodicity). ○

We now give an example for which $K_{\text{eff}} = K_{\text{Sachs}}$, showing the optimality of the Sachs bound.

Example 3. To simplify the notation, we depart from our usual convention by taking Q to be the unit cube centered at 0 rather than at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. Partition Q into six pyramids, each having its apex at the center of Q and its base at one face:

$$\begin{array}{ll} P_1 = \{x \in Q \;:\; x_3 \geq \max\{|x_1|, |x_2|\}\} & P_2 = \{x \in Q \;:\; -x_3 \geq \max\{|x_1|, |x_2|\}\} \\ P_3 = \{x \in Q \;:\; x_2 \geq \max\{|x_1|, |x_3|\}\} & P_4 = \{x \in Q \;:\; -x_2 \geq \max\{|x_1|, |x_3|\}\} \\ P_5 = \{x \in Q \;:\; x_1 \geq \max\{|x_2|, |x_3|\}\} & P_6 = \{x \in Q \;:\; -x_1 \geq \max\{|x_2|, |x_3|\}\}\,. \end{array}$$

Now consider a polycrystal such that

$R(x) = R_i$ is constant on each pyramid P_i, with $R_i e_1$ normal to the base of P_i.

Thus

$$R_i e_1 \text{ is parallel to } \begin{cases} e_3 & \text{for } i = 1, 2, \\ e_2 & \text{for } i = 3, 4, \\ e_1 & \text{for } i = 5, 6. \end{cases}$$

We claim that such a polycrystal has

$$K_{\text{eff}} = K_{\text{Sachs}} = \{\xi \;:\; |\xi|_\infty \leq 1\} \tag{3.4}$$

provided $M \geq \sqrt{2}$. To demonstrate this, we need merely show that

$$\xi \in K_{\text{eff}} \Longrightarrow |\xi_i| \leq 1 \text{ for } i = 1, 2, 3. \tag{3.5}$$

Indeed, (3.5) says $K_{\text{eff}} \subset \{\xi \;:\; |\xi|_\infty \leq 1\}$. But it is easy to check that $K_{\text{Sachs}} = \cap_{i=1}^6 R_i K_{M,N} = \{\xi \;:\; |\xi|_\infty \leq 1\}$ if $M \geq \sqrt{2}$, and we know in general that $K_{\text{Sachs}} \subset K_{\text{eff}}$, so (3.5) implies (3.4).

To prove (3.5) it suffices, by symmetry, to consider $i = 3$. If $\xi \in K_{\text{eff}}$ then there exists a Q-periodic, L^∞, divergence-free vector field σ such that $\sigma \in R(x) K_{M,N}$ and $\int_Q \sigma \, dx = \xi$. From Lemma 4 we have

$$|\xi_3| = \left| \int_{Q\cap\{x_3=t\}} \sigma_3 \, dx_1 \, dx_2 \right| \leq \int_{Q\cap\{x_3=t\}} |\sigma_3| \, dx_1 \, dx_2 \,. \tag{3.6}$$

for every $|t| \leq 1/2$. But for $x \in P_1$ we also have

$$|\sigma_3(x)| = |\langle \sigma, e_3 \rangle| = |\langle \sigma, R(x)e_1 \rangle| \leq 1 \tag{3.7}$$

since $\sigma \in R(x)K_{M,N}$. And by our choice of geometry, as $t \to 1/2$ the slice $Q \cap \{x_3 = t\}$ is almost entirely in P_1. Thus (3.6)-(3.7) give

$$|\xi_3| \leq \limsup_{t \to 1/2} \int_{P_1 \cap \{x_3 = t\}} |\sigma_3| \, dx_1 \, dx_2 \leq 1$$

as desired. ○

As usual, there is a lot of freedom in this construction. Indeed, our argument uses the choice of texture $R(x)$ at the faces. The argument really only requires that there be, for each i, a plane orthogonal to e_i along which the orientation satisfies $R(x)e_1 \| e_i$.

4 Conclusions

We have addressed two model problems motivated by polycrystal plasticity. One replaces the "stresses" by 3D gradient fields; the other replaces them by 3D divergence-free vector fields. In the first case the Taylor bound is far from optimal; in the second case it achieves the optimal scaling law. We conclude that the optimality of the Taylor bound (or at least its scaling law) depends strongly on (i) the dimensionality of the basic variable, and (ii) the character of the linear differential constraint.

For 3D gradients we have shown that the linear comparison method gives weaker results (at least in our implementation) than an argument based on the translation method using the 3D determinant. This calls into question the adequacy of linear comparison arguments for 3D problems.

Our results are most interesting when the yield domain of the basic crystal is highly eccentric, i.e. when $N \to \infty$. In this limit the Sachs and Taylor bounds are very different – the former is independent of N while the latter grows linearly with N. Our bounds and constructions suggest that while the Taylor bound can sometimes be improved, geometry-independent inner and outer bounds must necessarily be very far apart. They also give insight concerning the percolation character of the problem.

Bounds and constructions are important, because they (i) provide benchmarks for and restrictions upon any reasonable approximation scheme, and (ii) give insight concerning the behavior achievable via special textures. Bounds do not, however, help us identify the generic behavior. In particular, when the bounds are far apart they tell us rather little about the behavior of a specific polycrystal. Linear comparison methods, self-consistent schemes, and direct numerical simulation are presently the main tools for addressing generic behavior or specific composites, see e.g. [11, 13, 14]. We wonder, however, whether additional insight could be gained, for polycrystals with highly eccentric yield sets, through an analysis based on the intrinsic percolation-like character of the problem. The discussion in [5], though very preliminary, suggests an affirmative answer.

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