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Bounds on the hydrostatic plastic strength of voided polycrystals and implications for linear-comparison homogenization techniques

Bornes de la résistance plastique hydrostatique des polycrystaux poreux et leurs implications sur des techniques basées sur des milieux linéaires de comparaison

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ABSTRACT

A linear-comparison homogenization technique and its relaxed version are used to compute bounds of the Hashin–Shtrikman and the self-consistent types for the hydrostatic strength of ideally plastic voided polycrystals. Closed-form analytical results are derived for isotropic aggregates of various cubic symmetries (fcc, bcc, ionic). The impact of the variational relaxation on the bounds is found to be significantly larger than that previously observed in fully dense polycrystals. So much so that, quite surprisingly, relaxed self-consistent bounds are found to be weaker than non-relaxed Hashin–Shtrikman bounds in some of the material systems considered.

RÉSUMÉ

Une technique d'homogénéisation non linéaire et sa version relaxée sont utilisées pour calculer des bornes de types Hashin–Shtrikman et autocohérent pour la resistance hydrostatique de polycristaux poreux parfaitement plastiques. On en dérive des résultats analytiques pour des agrégats isotropes de différentes symétries cubiques (cfc, ccc, ionique). L'impact sur les bornes de la relaxation variationnelle se révèle être beaucoup plus important que celui précédemment observé dans le cas de polycristaux denses, tant et si bien que des bornes relaxées de type autocohérent s'avèrent être plus faibles que des bornes non relaxées de type Hashin–Shtrikman dans certains systèmes matériels considérés.

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1. Introduction

Several homogenization techniques are already available to bound the plastic strength of polycrystalline solids. The simplest bounds are the upper bound of Taylor [1] and the lower bound of Reuss [2], which depend on one-point microstructural statistics only. Sharper bounds incorporating higher-order statistics were first derived by Dendievel et al. [3] and deBotton and Ponte Castañeda [4] making use of the idea of a linear-comparison medium that is optimally selected via suitably designed variational principles. In particular, the technique of deBotton and Ponte Castañeda allows the use of any linear homogenization approach, such as the Hashin–Shtrikman or the self-consistent approach, to generate the corresponding results for nonlinear plastic polycrystals. Application of these linear-comparison techniques to various classes of fully dense polycrystalline solids have been pursued by Willis [5], Nebozhyn et al. [6,7], Liu et al. [8], and Liu and Ponte Castañeda [9]. In all cases, the nonlinear Hashin–Shtrikman bounds are very close to the Taylor bound, but the nonlinear self-consistent bounds can be quite sharper, especially for low-symmetry solids. This is in part due to the fact that the Hashin–Shtrikman results bound the entire class of polycrystals with prescribed one- and two-point statistics, while the self-consistent results bound the subclass of polycrystals that realize the linear self-consistent estimate.

Idiart and Ponte Castañeda [10,11] later showed that the linear-comparison technique of deBotton and Ponte Castañeda [4] makes implicit use of a relaxation in the variational scheme that weakens the resulting bounds. Eliminating this relaxation leads to sharper bounds at the expense of increasing the computational complexity. The impact of the relaxation in the context of various cubic and hexagonal systems has been recently assessed by Idiart [12]. Modest differences between relaxed and non-relaxed bounds were observed, with the largest amounts corresponding to materials with deficient slip systems. Given that these are materials with a strong heterogeneity contrast, the question arises as to whether larger differences will appear in the context of (two-phase) polycrystalline voided solids where the heterogeneity contrast is infinitely strong. This Note reports linear-comparison bounds of the Hashin–Shtrikman and self-consistent types for the plastic strength of polycrystalline voided solids exhibiting overall isotropic symmetry and subjected to purely hydrostatic loadings. These conditions are of particular theoretical interest since they usually exacerbate differences between theories and, furthermore, allow analytical treatment. It turns out that the impact of the relaxation on the bounds can be significantly larger than that observed in fully dense polycrystals. So much so that, quite surprisingly, relaxed self-consistent bounds are found to be weaker than non-relaxed Hashin–Shtrikman bounds for some of the material systems considered. We conclude the Note by discussing some implications for the use of linear-comparison techniques in the context of voided polycrystals.

2. The polycrystalline solid model

Polycrystals are taken here as random aggregates of perfectly bonded single crystals (i.e., grains) and voids. Following Lebensohn et al. [13], individual grains and voids are assumed to be of a similar size, much smaller than the specimen size and the scale of variation of the applied loads. Grain orientations are characterized by rotation tensors $\mathbf{Q}^{(r)}$ $(r = 1, \ldots, N)$. All grains with a given orientation $\mathbf{Q}^{(r)}$ occupy a disconnected domain $\Omega^{(r)}$ and are collectively referred to as 'phase' r. Similarly, all voids occupy a disconnected domain $\Omega^{(0)}$ and are collectively referred to as 'phase' 0.

Grains are assumed to deform by multi-glide along K slip systems following a rigid-perfectly plastic response. In accordance with standard crystal plasticity theory, their *strength domains* are characterized in terms of a convex set:

$$P = \left\{\boldsymbol{\sigma}\colon\ |\boldsymbol{\sigma}\cdot\boldsymbol{\mu}_{(k)}| \leqslant \tau_0^{(k)},\ k = 1, \ldots, K\right\} \tag{1}$$

where $\tau_0^{(k)} > 0$ is the yield strength of the kth slip system and:

$$\boldsymbol{\mu}_{(k)} = \frac{1}{2}(\mathbf{n}_{(k)} \otimes \mathbf{m}_{(k)} + \mathbf{m}_{(k)} \otimes \mathbf{n}_{(k)}) \tag{2}$$

are second-order Schmid tensors with $\mathbf{n}_{(k)}$ and $\mathbf{m}_{(k)}$ denoting the unit vectors normal to the slip plane and along the slip direction of the kth system in a 'reference' crystal, respectively. Note that the Schmid tensors are traceless and therefore the strength domains (1) are insensitive to hydrostatic stresses. The set P is a convex polyhedron formed by the set of planes (or facets) whose equations are given by the equalities in (1). The set of vertices of P is denoted as $\hat{P}$. The strength domain $P^{(r)}$ of phase r is given by a set similarly defined in terms of rotated Schmid tensors $\boldsymbol{\mu}_{(k)}^{(r)} = \mathbf{Q}^{(r)^T}\boldsymbol{\mu}_{(k)}\mathbf{Q}^{(r)}$. The boundary $\partial P^{(r)}$ of the set $P^{(r)}$ represents the *yield surface* of phase r. The voided phase $(r = 0)$, on the other hand, cannot sustain stress. We characterize this phase as a family of 'grains' with $P^{(0)} = \{\mathbf{0}\}$.

The macroscopic plastic strength of the polycrystalline aggregate corresponds to the set of stress states that can produce macroscopic plastic flow. By homogenizing the relevant field equations, Suquet [14] and Bouchitté and Suquet [15] showed that the macroscopic plastic strength can be characterized by an *effective strength domain* defined as:

$$\widetilde{P} = \left\{\bar{\boldsymbol{\sigma}}\colon\ \exists\boldsymbol{\sigma}(\mathbf{x}) \in \mathcal{S}(\bar{\boldsymbol{\sigma}}) \text{ and } \boldsymbol{\sigma}(\mathbf{x}) \in P^{(r)} \text{ in } \Omega^{(r)},\ r = 0, \ldots, N\right\} \tag{3}$$

where $\bar{\boldsymbol{\sigma}}$ denote the macroscopic stress states, $\boldsymbol{\sigma}(\mathbf{x})$ are the underlying microscopic stress fields, and $\mathcal{S}(\bar{\boldsymbol{\sigma}})$ denotes the set of statically admissible stress fields with volume average $\bar{\boldsymbol{\sigma}}$. The effective strength domain depends on the *crystallographic* texture of the polycrystal through the set of orientations $\mathbf{Q}^{(r)}$, and on the *morphological* texture and porosity through the ensemble averages of the characteristic functions of the domains $\Omega^{(r)}$. The boundary $\partial\widetilde{P}$ of the set $\widetilde{P}$ represents the *effective yield surface* of the polycrystalline voided solid.

3. Linear-comparison bounds

The linear-comparison technique given in Idiart and Ponte Castañeda [10,11] is used here to generate outer bounds on the effective strength domain (3). The main idea behind the technique is to introduce a comparison polycrystal with the same microstructural domains $\Omega^{(r)}$ as the original polycrystal but with linear stress-strain-rate local responses characterized by a positive-semidefinite,[1] incompressible, symmetric compliance tensors $\mathbb{S}^{(r)}$. The resulting bound is given by:

$$\widetilde{P} \subset \widetilde{P}_+ = \left\{\bar{\boldsymbol{\sigma}}\colon \tilde{u}\left(\bar{\boldsymbol{\sigma}};\mathbb{S}^{(s)}\right) \leqslant v\left(\mathbb{S}^{(s)}\right), \forall \mathbb{S}^{(r)} \geqslant 0\ (r=1,\ldots,N)\right\} \tag{4}$$

where

$$\tilde{u}\left(\bar{\boldsymbol{\sigma}};\mathbb{S}^{(s)}\right) = (1-f)\min_{\boldsymbol{\sigma}\in\mathcal{S}^*(\bar{\boldsymbol{\sigma}})}\sum_{r=1}^{N} c_g^{(r)}\left\langle\frac{1}{2}\boldsymbol{\sigma}\cdot\mathbb{S}^{(r)}\boldsymbol{\sigma}\right\rangle^{(r)} \tag{5}$$

$$v\left(\mathbb{S}^{(s)}\right) = (1-f)\sum_{r=1}^{N} c_g^{(r)} v^{(r)}\left(\mathbb{S}^{(r)}\right) \tag{6}$$

and

$$v^{(r)}\left(\mathbb{S}^{(r)}\right) = \sup_{\boldsymbol{\sigma}\in P^{(r)}}\frac{1}{2}\boldsymbol{\sigma}\cdot\mathbb{S}^{(r)}\boldsymbol{\sigma} = \max_{\boldsymbol{\sigma}\in\hat{P}^{(r)}}\left\{\frac{1}{2}\boldsymbol{\sigma}\cdot\mathbb{S}^{(r)}\boldsymbol{\sigma}\right\} \tag{7}$$

In these expressions, $\tilde{u}$ represents the effective stress potential of the linear-comparison polycrystal, while the functions $v^{(r)}$ represent a measure of the non-linearity of the local stress-strain-rate plastic relation. In turn, the set $\mathcal{S}^* \subset \mathcal{S}$ denotes the subset of statically admissible stress fields with zero traction on the surfaces $\partial\Omega^{(0)}$ of the voids, f is the volume of fraction of voids or porosity, and $c_g^{(r)}$ is the volume fraction of each phase r in the polycrystalline matrix, such that $\sum_{r=1}^{N} c_g^{(r)} = 1$—see Ref. [13]. The last equality in (7) follows from a well-known theorem of convex analysis [16]; note that the maximizations in the $v^{(r)}$'s reduce thus to evaluating the objective function over a finite set of points. The boundary of $\widetilde{P}_+$ represents a surface in the space of macroscopic stresses that bounds from outside the effective yield surface of the polycrystalline voided solid; it can be written as:

$$\partial\widetilde{P}_+ = \left\{\bar{\boldsymbol{\sigma}}\colon \bar{\boldsymbol{\sigma}} = \Lambda\overline{\boldsymbol{\Sigma}} \text{ with } \|\overline{\boldsymbol{\Sigma}}\| = 1 \text{ and } \Lambda = \inf_{\mathbb{S}^{(r)}\geqslant 0}\left(\frac{\tilde{u}(\overline{\boldsymbol{\Sigma}};\mathbb{S}^{(s)})}{v(\mathbb{S}^{(s)})}\right)^{-1/2}\right\} \tag{8}$$

where $\|\cdot\|$ denotes the Euclidean norm of a tensor. The reader is referred to the work of Idiart and Ponte Castañeda [10]—Section 4b—for details on the derivation.

3.1. Relaxations

The computation of the bound (8) can be simplified by restricting the set of compliance tensors $\mathbb{S}^{(r)}$ to those of the form:

$$\mathbb{S}^{(r)} = 2\sum_{k=1}^{K}\alpha_{(k)}^{(r)}\boldsymbol{\mu}_{(k)}^{(r)}\otimes\boldsymbol{\mu}_{(k)}^{(r)}, \quad \alpha_{(k)}^{(r)} \geqslant 0 \tag{9}$$

where the $\boldsymbol{\mu}_{(k)}^{(r)}$ are the Schmid tensors of the crystalline phase r and the scalar variables $\alpha_{(k)}^{(r)}$ represent slip compliances. This class of compliance tensors arise naturally in the linear-comparison bounds of deBotton and Ponte Castañeda [4]; they facilitate the computation of the function v and the optimization with respect to the linear-comparison properties. As a result of the restriction (9), we obtain a weaker bound $\partial\widetilde{P}'_+$ such that $\widetilde{P}_+ \subset \widetilde{P}'_+$. We will refer to this bound as *relaxed*.

A further simplification results upon use of the inequality:

$$v^{(r)}\left(\mathbb{S}^{(r)}\right) = \sup_{\boldsymbol{\sigma}\in P^{(r)}}\frac{1}{2}\boldsymbol{\sigma}\cdot\mathbb{S}^{(r)}\boldsymbol{\sigma} \leqslant \sum_{k=1}^{K}\alpha_{(k)}^{(r)}\left(\tau_0^{(k)}\right)^2 \doteq v^{(r)''}\left(\alpha_{(k)}^{(r)}\right) \tag{10}$$

to replace the function v in (8) by a relaxed function v'' similarly defined in terms of the above functions $v^{(r)''}$; the result can be written as:

$$\partial\widetilde{P}''_+ = \left\{\bar{\boldsymbol{\sigma}}\colon \bar{\boldsymbol{\sigma}} = \Lambda\overline{\boldsymbol{\Sigma}} \text{ with } \|\overline{\boldsymbol{\Sigma}}\| = 1 \text{ and } \Lambda = \inf_{\alpha_{(k)}^{(r)}\geqslant 0}\left(\frac{\tilde{u}(\overline{\boldsymbol{\Sigma}};\alpha_{(k)}^{(s)})}{v''(\alpha_{(k)}^{(s)})}\right)^{-1/2}\right\} \tag{11}$$

[1] Positive-semidefiniteness of a fourth-order tensor $\mathbb{S}$ will be indicated by the inequality $\mathbb{S} \geqslant 0$.

The sense of the inequality (10) implies that $\partial\widetilde{P}''_+$ is such that $\widetilde{P}_+ \subset \widetilde{P}'_+ \subset \widetilde{P}''_+$. This weaker bound agrees exactly with the bound originally derived by deBotton and Ponte Castañeda [4]. We will refer to this bound as *fully relaxed*. Note that the inequality in (10) becomes an equality when the total number of slip systems at the single-crystal level is five and all of them are linearly independent [11]: in this case, the bounds $\partial\widetilde{P}'_+$ and $\partial\widetilde{P}''_+$ coincide.

4. Application to isotropic cubic polycrystals under hydrostatic loadings

With the purpose of assessing the impact of the variational relaxation on the resulting bounds, the non-relaxed and fully relaxed bounds are applied here to voided polycrystals with isotropic microstructural statistics, subjected to hydrostatic loadings. For simplicity, we restrict our attention to cubic materials with $\tau_0^{(k)} = \tau_0$ for all slip systems.

4.1. Non-relaxed bounds

The hydrostatic stress $\bar{\boldsymbol{\sigma}}_h$ belonging to the bounding yield surface (8) is given by:

$$\bar{\boldsymbol{\sigma}}_h = \bar{\sigma}_h \mathbf{I} = \Lambda_h \overline{\boldsymbol{\Sigma}}_h \quad \text{with} \quad \overline{\boldsymbol{\Sigma}}_h = \frac{1}{\sqrt{3}}\mathbf{I} \quad \text{and} \quad \Lambda_h = \inf_{\mathbb{S}^{(r)} \geqslant 0} \left(\frac{\tilde{u}(\overline{\boldsymbol{\Sigma}}_h; \mathbb{S}^{(s)})}{v(\mathbb{S}^{(s)})} \right)^{-1/2} \tag{12}$$

where $\bar{\sigma}_h$ is an *upper* bound for the hydrostatic strength. Owing to the overall spherical symmetry of the microstructure and the loading, the linear-comparison polycrystal must be isotropic and the optimal compliance tensors $\mathbb{S}^{(r)}$ must be all $\mathbf{Q}^{(r)}$-rotations of a single tensor $\hat{\mathbb{S}}$; therefore, we can write:

$$\tilde{u}(\overline{\boldsymbol{\Sigma}}_h; \hat{\mathbb{S}}) = \frac{1}{6\tilde{\kappa}(\hat{\mathbb{S}})} \quad \text{and} \quad v(\hat{\mathbb{S}}) = (1-f)\hat{v}(\hat{\mathbb{S}}) \tag{13}$$

where $\hat{v}$ is given by expression (7) with $P^{(r)}$ replaced by P, and $\tilde{\kappa}$ is the bulk modulus of the linear-comparison polycrystal. The expression for $\tilde{\kappa}$ depends on the specific choice of linear homogenization approach. In this work we consider the Hashin–Shtrikman (HS) and self-consistent (SC) approaches as given by Willis [17,18]. When specialized to our linear-comparison polycrystal, they yield the expression:

$$\tilde{\kappa}(\hat{\mathbb{S}}) = \frac{4}{3}\frac{1-f}{f}\mu_0(\hat{\mathbb{S}}) \tag{14}$$

where μ_0 is a reference shear modulus dictated by the prescriptions

$$\mu_0(\hat{\mathbb{S}}) = \begin{cases} \frac{1}{2}\|\hat{\mathbb{S}}^{-1}\|_2 & \text{HS} \\ \tilde{\mu}(\hat{\mathbb{S}}) \text{ where } \mathbb{K}\cdot[\mathbb{K} + 2\tilde{\mu}\frac{3-f}{2+f}\hat{\mathbb{S}}]^{-1} - \frac{2+f}{1-f} = 0 & \text{SC} \end{cases} \tag{15}$$

In these expressions, $\tilde{\mu}$ denotes the effective shear modulus of the linear-comparison polycrystal, $\mathbb{K}$ is the standard, fourth-order, incompressible projection tensor, and the norm $\|\cdot\|_2$ delivers the maximum eigenvalue of a tensor.

Now, owing to the cubic symmetry of the crystals, the optimal tensor $\hat{\mathbb{S}}$ must be of the form:

$$\hat{\mathbb{S}} = \frac{1}{2\mu_a}\mathbb{K}_a + \frac{1}{2\mu_s}\mathbb{K}_s = \frac{1}{2\mu_s}\left[\frac{1}{r}\mathbb{K}_a + \mathbb{K}_s\right] \tag{16}$$

where $r \doteq \mu_a/\mu_s$ is a cubic anisotropy ratio, and the tensors $\mathbb{K}_a$ and $\mathbb{K}_s$ denote the incompressible, fourth-order, cubic projections [19]:

$$\mathbb{K}_a = \mathbb{T} - \mathbb{J} \quad \text{and} \quad \mathbb{K}_s = \mathbb{K} - \mathbb{K}_a \tag{17}$$

here, $\mathbb{J}$ is the standard, fourth-order, hydrostatic projection tensor and $\mathbb{T}$ has components relative to the cubic symmetry axes $\mathbb{T}_{ijkl} = 1$ if $i = j = k = l$ and $\mathbb{T}_{ijkl} = 0$ otherwise. For this class of compliance tensors, the function $\hat{v}$ can be written as:

$$\hat{v}(\hat{\mathbb{S}}) = \frac{\tau_0^2}{2\mu_s}\max_{\boldsymbol{\sigma}\in\hat{P}}\left\{\frac{1}{2}\left(\tau_0^{-1}\boldsymbol{\sigma}\right)\cdot\left[\frac{1}{r}\mathbb{K}_a + \mathbb{K}_s\right]\left(\tau_0^{-1}\boldsymbol{\sigma}\right)\right\} \doteq \frac{\tau_0^2}{2\mu_s}\hat{v}(r) \tag{18}$$

while the prescriptions (15) for the reference modulus can be written as $\mu_0 = m_0(r, f)\mu_s$ with:

$$m_0(r,f) = \begin{cases} \max\{1, r\} & \text{HS} \\ \frac{1-4f-3fr+\sqrt{(1-4f)^2+6(4-7f)r+9f^2r^2}}{2(3-f)} & \text{SC} \end{cases} \tag{19}$$

Introducing these expressions into (12), we obtain:

$$\frac{\bar{\sigma}_h}{\tau_0} = \frac{2}{\sqrt{3}}\frac{1-f}{\sqrt{f}}\sqrt{g(f)} \tag{20}$$

where

$$g(f) = \inf_{r\geqslant 0}\left[m_0(r,f)\,\hat{v}(r)\right] \tag{21}$$

4.2. Fully relaxed bounds

The hydrostatic stress $\bar{\boldsymbol{\sigma}}_h$ belonging to the bounding yield surface (11) is given by an expression analogous to (12) with the function $v(\mathbb{S}^{(s)})$ replaced by $v''(\alpha_{(k)}^{(s)})$. Once again, owing to the overall spherical symmetry of the microstructure and the loading, the linear-comparison polycrystal must be isotropic and the compliance tensors associated with the set of optimal $\alpha_{(k)}^{(r)}$'s must be all $\mathbf{Q}^{(r)}$-rotations of a single compliance tensor with cubic symmetry. Hashin–Shtrikman and self-consistent bounds can be obtained by derivations analogous to those of the previous subsection; the result can be written as (20), with:

$$g(f) = \inf_{\alpha_{(k)} \geqslant 0} \left[m_0(r, f)\, \hat{v}''(\alpha_{(k)}) \right] \tag{22}$$

In this expression, $m_0(r, f)$ is the same function (19), $\hat{v}'' \doteq 2\mu_s v''/\tau_0^2$, and:

$$r = \frac{2}{3} \frac{\sum_{k=1}^{K} \alpha_{(k)} \boldsymbol{\mu}_{(k)} \cdot \mathbb{K}_s \boldsymbol{\mu}_{(k)}}{\sum_{k=1}^{K} \alpha_{(k)} \boldsymbol{\mu}_{(k)} \cdot \mathbb{K}_a \boldsymbol{\mu}_{(k)}} \quad \text{and} \quad \hat{v}''(\alpha_{(k)}) = \frac{3}{2} \frac{\sum_{k=1}^{K} \alpha_{(k)}}{\sum_{k=1}^{K} \alpha_{(k)} \boldsymbol{\mu}_{(k)} \cdot \mathbb{K}_s \boldsymbol{\mu}_{(k)}} \tag{23}$$

The mathematical structure of the objective function in (22) implies that the optimal slip compliances $\alpha_{(k)}$ associated with all those slip systems with equal projections $\boldsymbol{\mu}_{(k)} \cdot \mathbb{K}_s \boldsymbol{\mu}_{(k)}$ and $\boldsymbol{\mu}_{(k)} \cdot \mathbb{K}_a \boldsymbol{\mu}_{(k)}$ will take the same values. Note also that the objective function is homogeneous of degree zero in the slip compliances.

4.3. Results and discussion for specific material systems

In this section, we report bounds for three types of cubic material systems:

- Face-centered cubic (fcc) solids that deform plastically on a set of four slip planes of the type {111} along three slip directions (per plane) of type ⟨110⟩, which constitute a set of twelve slip systems ($K = 12$). This set of slip systems defines a yield surface with fifty-six vertices.
- Body-centered cubic (bcc) solids that deform through slip along the ⟨111⟩ directions on the {110} and {112} planes—pencil glide along {123} planes is not considered—, which constitute a set of twenty-four slip systems ($K = 24$). This set of slip systems defines a yield surface with four hundred and thirty-two vertices.
- Ionic solids that deform plastically on three different families of slip systems: {110}⟨110⟩, {100}⟨110⟩, {111}⟨110⟩. Each one of the first two families consists of six systems, while the last family consists of the same twelve slip systems of an fcc crystal. The three families together consist of twenty-four slip systems ($K = 24$) and define a yield surface with three hundred and twelve vertices.

Hashin–Shtrikman and self-consistent bounds for these material systems are obtained by solving the optimization problems in (21) and (22); the resulting functions $g(f)$ are given by:

$$\text{fcc:} \quad g(f) = \begin{cases} 6 & \text{HS} \\ 9 & \text{HS}'' \\ \frac{1-5f+\sqrt{9-22f+17f^2}}{1-f/3} & \text{SC} \\ \frac{3}{2}\frac{1-5f+\sqrt{9-22f+17f^2}}{1-f/3} & \text{SC}'' \end{cases} \tag{24}$$

$$\text{bcc:} \quad g(f) = \begin{cases} 3(5-2\sqrt{3}) & \text{HS} \\ 9 & \text{HS}'' \\ 3(2-\sqrt{3})\frac{1-5f+\sqrt{9-22f+17f^2}}{1-f/3} & \text{SC} \\ \frac{3}{2}\frac{1-5f+\sqrt{9-22f+17f^2}}{1-f/3} & \text{SC}'' \end{cases} \tag{25}$$

$$\text{ionic:} \quad g(f) = \begin{cases} 3 & \text{HS} \\ 5 & \text{HS}'' \\ 3\frac{1-2f}{1-f/3} & \text{SC} \\ 5\frac{1-2f}{1-f/3} & \text{SC}'' \end{cases} \tag{26}$$

where it is recalled that unprimed and double-primed labels refer to non-relaxed and fully relaxed bounds, respectively. The above bounds of the self-consistent type are all valid in the range $0 \leqslant f \leqslant 1/2$. The SC bound for ionic materials given in (26) is not exact, but it approximates the exact result to a high degree of accuracy and proves convenient for comparison purposes.

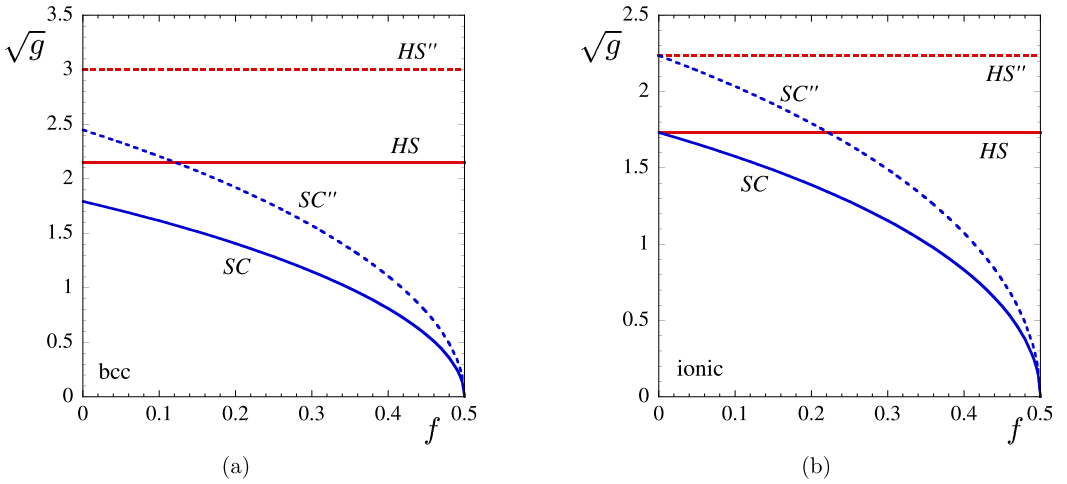

Fig. 1. Linear-comparison bounds of the Hashin–Shtrikman (HS) and self-consistent (SC) type for the hydrostatic strength of isotropic voided polycrystals as a function of the porosity f: (a) bcc materials, (b) ionic materials. Unprimed and double-primed labels refer to non-relaxed and relaxed bounds, respectively.

Several comments regarding these results are in order. We begin by recalling that the elementary bounds of Taylor and Reuss become trivial—infinite and identically zero, respectively—in the present context. In contrast, the above linear-comparison bounds are all finite, except at percolation. The percolation thresholds in HS and SC results are $f = 1$ and $f = 1/2$, respectively. The variational relaxation has a detrimental impact on the bounds in all cases considered. This impact is independent of the porosity level, and it is smallest in fcc materials (∼22%), intermediate in ionic materials (∼29%), and largest in bcc materials (∼40%).[2] In any case, it is significantly larger than that previously observed by Idiart [12] in fully dense polycrystalline solids (<15%). In addition, the relaxation seems to reduce the sensitivity of the bounds to matrix crystallinity: the relaxed bounds do not distinguish between fcc and bcc materials, cf. expressions (24) and (25).

More surprisingly, however, is the fact that, in addition to being weaker than their non-relaxed counterparts as expected, the relaxed self-consistent bounds can be weaker than the non-relaxed Hashin–Shtrikman ones. Fig. 1 shows plots for the various bounds corresponding to bcc and ionic materials as a function of porosity. Indeed, it is observed that below certain porosity levels, the SC″ results lie above the HS results by as much as 30% in the case of ionic materials with infinitesimally low porosity levels. Recall that the HS results constitute rigorous upper bounds for all other results, including the SC″ results.

The above observations may be exploited in current efforts to develop polycrystalline theories of dilatational plasticity via linear-comparison techniques [13]. These techniques are typically used in conjunction with a linear self-consistent approximation, for it is well known that this approximation delivers accurate estimates for linear polycrystalline solids. In contrast, the use of a linear Hashin–Shtrikman approximation is usually discarded for it presumably delivers exceedingly 'stiff' predictions. While this is indeed the case in the context of fully dense polycrystals, the above results suggest that it may not be the case in the context of voided polycrystals with low porosity levels, which is precisely the porosity range of interest in applications such as ductile failure of metals and forming processes. The use of a Hashin–Shtrikman approximation instead of a self-consistent one could prove advantageous from a practical standpoint in view of the lower computational demands of the Hashin–Shtrikman approximation. The choice is likely to depend, however, on the performance of the various approximations for more general (viscoplastic) constitutive responses and (non-spherical) loading conditions. In this connection, it is recalled that linear-comparison estimates for voided systems are known to be fairly accurate for low to moderate stress triaxialities, but are unrealistic at high triaxialities [13]. While the improvements found in this work are not expected to render the estimates for hydrostatic loadings realistic, they are expected to enlarge the range of stress triaxialities for which the estimates are accurate. An assessment is currently being pursued and will be reported upon completion.

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