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Hill–Mandel condition and bounds on lower symmetry elastic crystals

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ABSTRACT

Despite advances in contemporary micromechanics, there is a void in the literature on a versatile method for estimating the effective properties of polycrystals comprising of highly anisotropic single crystals belonging to lower symmetry class. Basing on variational principles in elasticity and the Hill–Mandel homogenization condition, we propose a versatile methodology to fill this void. It is demonstrated that the bounds obtained using the Hill–Mandel condition are tighter than the Voigt and Reuss [1,2] bounds, the Hashin–Shtrikman [3] bounds as well as a recently proposed self-consistent estimate by Kube and Arguelles [4] even for polycrystals with highly anisotropic single crystals.

1. Introduction

Polycrystalline materials are widely used in engineering applications as the need to develop new materials with unique properties has significantly increased (enhanced fracture toughness [5], high thermal conductivity [6], superior electrical conductivity [7]). These microstructures consist of collection of single crystals with random orientations and individual grains belonging to any crystal class (from cubic to triclinic). When these crystals are oriented randomly, collectively they exhibit an effective elastic behavior that is isotropic upon ensemble averaging. However, despite advances in contemporary micromechanics over the past several decades, it is still a challenge to predict the effective properties of such polycrystals especially when the single crystals are highly anisotropic and have lower elastic symmetry (see [8,9,4]).

In the past, several techniques have been used to predict the elastic response of materials and some of these are noteworthy. Voigt [1] developed the upper bound on the elastic moduli by assuming uniform strain throughout the material. Along similar lines, Reuss [2] obtained the lower bound on the aggregate response by considering uniform stress in the composite. It was later demonstrated by Hashin–Shtrikman [3] using variational principles that the upper and lower bounds for the elastic moduli of polycrystals can be tighter than the Voigt and Reuss bounds. Also, the authors applied their approach to a two-phase alloy that had cubic symmetry and illustrated that the theoretical results were in good agreement with the experimental results. Several other authors had employed Hashin–Shtrikman's variational principles method for polycrystals from various crystal classes. In particular, Watt and Peselnick [10] demonstrated explicit expressions for the bounds on the elastic moduli of polycrystalline aggregates composed of hexagonal, trigonal and tetragonal crystals. Also, the authors showed that Hashin–Shtrikman bounds were within the Voigt and Reuss bounds. Similarly, Berryman [11] developed analytical formulas in order to obtain self-consistent estimates for the shear and bulk moduli of random polycrystals with hexagonal, trigonal and tetragonal symmetries. In addition, the author was successful in obtaining the self-consistent estimates within the Hashin–Shtrikman bounds for all the crystal classes considered in that study.

An alternate approach for estimating the effective property is the Mori–Tanaka method which relates the average stress in an inclusion to the average stress in the matrix in multiphase composites. In particular, Norris [12] investigated two phase composites and proved that the elastic moduli obtained using Mori–Tanaka method always satisfied the Hashin–Shtrikman bounds. Also, for spherical particles, it was demonstrated that the results for the effective moduli of multiphase composites were within the Hashin–Shtrikman bounds.

While several theories exist in the literature for determining the elastic response of materials, somewhat tighter bounds for elastic constants have only been recently obtained for microstructures with lower symmetry. In particular, Brown [13] illustrated a numerical technique for obtaining the Hashin–Shtrikman bounds for materials belonging to any crystal class. In that study, the author estimated the Hashin–Shtrikman bounds as a function of the prop-

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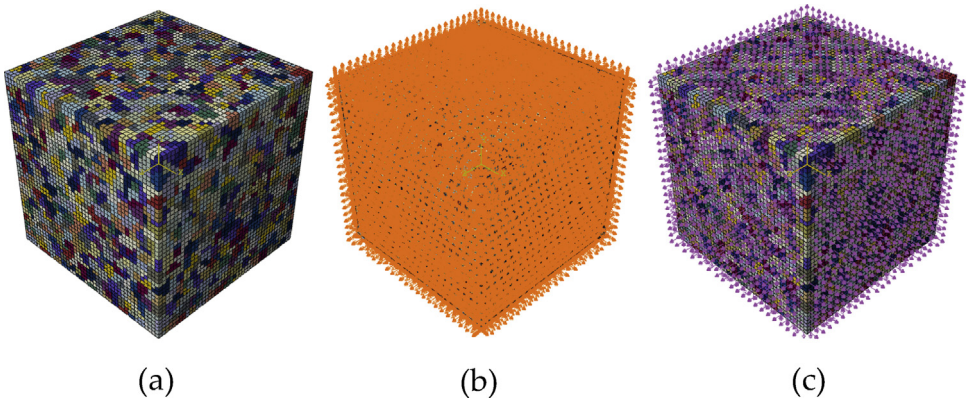

Fig. 1. (a) Microstructure of a polycrystal with 10,000 grains. (b) Microstructure subjected to Dirichlet boundary condition. (c) Microstructure subjected to Neumann boundary condition.

Table 1
Bounds (Voigt(V)–Reuss(R), Hashin–Shtrikman (HS), Dirichlet(d)–Neumann(t)) and self-consistent estimates (SC) of the shear (μ) moduli (GPa)

Material	A^U	μ^R	$\mu^- HS$	μ^t	Kube and Arguelles [4], μ^{SC}	μ^d	$\mu^+ HS$	μ^V	$\frac{\mu^{SC}-\mu^t}{\mu^{SC}} \times 100$	$\frac{\mu^{SC}-\mu^d}{\mu^{SC}} \times 100$
An_{96} (triclinic)	1.00	35.70	38.20	38.95	38.90	39.33	39.70	42.50	−0.13	−1.10
Tin difluoride (monoclinic)	1.80	10.30	11.60	12.12	12.10	12.39	12.40	13.80	−0.15	−2.38
Ethylene diamine tartrate (monoclinic)	2.80	6.20	7.00	7.13	7.10	7.31	7.70	9.10	−0.47	−2.91
Oxalic acid dihydrate (monoclinic)	3.60	4.20	4.90	5.44	5.40	5.59	5.80	6.90	−0.82	−3.58
Lithium hydrogen oxalate monohydrate (triclinic)	4.50	11.50	14.00	15.17	15.00	15.73	16.90	20.10	−1.14	−4.84

Table 2
Bounds (Voigt(V)–Reuss(R), Hashin–Shtrikman (HS), Dirichlet(d)–Neumann(t)) and self-consistent estimates (SC) of the bulk (κ) moduli (GPa)

Material	A^U	κ^R	$\kappa^- HS$	κ^t	Kube & Arguelles [4], κ^{SC}	κ^d	$\kappa^+ HS$	κ^V	$\frac{\kappa^{SC}-\kappa^t}{\kappa^{SC}} \times 100$	$\frac{\kappa^{SC}-\kappa^d}{\kappa^{SC}} \times 100$
An_{96}	1.00	84.10	86.20	86.71	86.70	87.01	87.20	88.70	−0.01	−0.36
Tin difluoride	1.80	16.50	17.10	17.36	17.30	17.44	17.50	17.90	−0.33	−0.81
Ethylene diamine tartrate	2.80	15.90	19.20	19.63	19.50	20.27	21.30	24.50	−0.64	−3.93
Oxalic acid dihydrate	3.60	10.80	11.90	12.46	12.40	12.70	13.00	14.30	−0.44	−2.44
Lithium hydrogen oxalate monohydrate	4.50	22.10	27.50	29.83	29.70	31.11	33.20	39.30	−0.44	−4.75

erties of a reference isotropic material and reported the results for crystals with triclinic symmetry. Following Brown's [13] computational procedure, Kube and Arguelles [4] developed theoretical expressions for obtaining the self-consistent estimates of polycrystals and illustrated an iterative approach to solve these expressions. It was seen that the estimates can be obtained for a variety of geological materials that have monoclinic and triclinic symmetries.

In the present work, we illustrate an alternate method for obtaining tighter bounds than Kube and Arguelles [4] using the Hill–Mandel condition (see Hill [14] and Mandel [15]). This approach has been widely used in the past few decades within the context of elasticity [8,9,16,17], thermal conductivity [18–21], thermoelasticity [22,23], electrical conductivity [24], fracture and damage phenomena in random microstructures [25], flow in porous media [26,27], viscoelastic materials [28] and nonlinear elastic and inelastic materials [29–31]. Proceeding with this framework, we analyze the mesoscale constitutive response of elastic polycrystals with increasing length scales by applying boundary conditions (displacement and traction) consistent with the Hill–Mandel condition. In this approach, one requires the polycrystals to be spatially homogeneous, ergodic and the applied boundary conditions to be macroscopically uniform so that the aggregate response is independent of the surface values of displacement and traction. Therefore, the microstructure moves from being a statistical volume element (SVE) to a representative volume element (RVE) with a growing length scale and the SVE's response becomes independent of the boundary conditions. Thus, displacement (Dirichlet) and traction (Neumann) boundary value problems deliver rigorous bounds on the effective elastic moduli from above and below, respectively.

In the subsequent sections, we establish scale-dependent bounds on the elastic response of random polycrystals with 10,000 grains which were generated using Voronoi Tessellations. By analyzing stochastic boundary value problems (Dirichlet and Neumann) consistent with the Hill–Mandel condition, we illustrate that the aggregate response of polycrystals converge to the effective properties. Subsequently, tighter bounds are obtained than the bounds and self-consistent estimates published in the literature by Voigt and Reuss [1,2], Hashin–Shtrikman [3] and Kube and Arguelles [4].

2. Mathematical formulation

2.1. Hill–Mandel condition

In this section, we illustrate the Hill–Mandel condition that employs the energetic and mechanistic approaches for setting up constitutive equations (see Hill [14] and Mandel [15]). Firstly, we discuss the stress and strain fields ($\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$) and decompose