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Microstructures by design: linear problems in elastic–plastic design

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Abstract

Materials microstructure is considered to be a design variable in the methodology called microstructure sensitive design (MSD). Based upon existing homogenization relations, relating the first-order representation of microstructure (the local state distribution function) to elastic and yield properties, the paper describes the construction of properties closures. These establish the theoretically-possible combinations of properties achievable by the set of all possible microstructures, which is called the microstructure hull. Exemplary homogenization relations are shown to be, typically, hypersurfaces (often hyperplanes) in the Fourier space in which the microstructure hull resides. All points lying on (or to one side of) the hypersurface, that also intersects the microstructure hull, represent microstructures that are predicted to have the same property (or property bound). It follows that intersections of several hypersurfaces (representing several properties), with the microstructure hull, represent allowable combinations of properties. From these intersections, combined properties closures have been constructed using conventional methods of linear programming. The primary example chosen is the cubic–orthorhombic Cu–Ni alloy system; for this case the elastic properties reside in a three-dimensional subspace of the infinite dimensional microstructure hull, and therefore a graphical depiction of the problem is convenient.

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1. Introduction

Materials science and engineering has long aimed to develop accurate relationships between the combinations of properties required by engineers/designers, the

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microstructures that realize them, and the set of manufacturing processes that induce the appropriate microstructures in the material. The focus of this paper is the ‘front end’ of microstructure design; namely, we seek to describe the set of all combinations of properties that are theoretically-achievable by varying microstructure over all of its possibilities, without explicit concern over how these microstructures might be achieved by tailored processing.

In this paper we enlarge upon the spectral method of microstructure design, suggested in the work of Bunge (1982), and developed in the paper of Adams et al. (2001). The methodology, called microstructure sensitive design (MSD), emphasizes basic mechanical properties that are linear (or mildly nonlinear) in their functional dependence upon the quantitative descriptors of microstructure. When the basic functional dependence is linear, it is convenient to solve the microstructure design problem in a carefully-chosen Fourier framework. Other methods that may be applied when the properties or performance criteria are nonlinear in their functional dependence upon the pertinent descriptors are described in Henrie et al. (2002). The focus of this paper is the concept of *properties and performance closures*. These provide a useful linkage between the materials engineer/scientist and the world of the designer, who is frequently called upon to balance multiple design objectives/constraints with available properties. The emphasis of the paper is on basic properties that impact mechanical design.

The linear MSD methodology makes use of descriptions of microstructure and structure-properties relationships in a Fourier space. The pertinent structure-properties relationships are taken from the generalized composite theory that has been developed extensively during the past five decades. Extensive reviews of the homogenization relationships of generalized composite theory, with an emphasis on two-phase composites, have been published by Milton (2002), Torquato (2002), and Cherkaev (2000). Adams and Olson (1998) reviewed applications of the theory, with a focus on polycrystalline materials. Generalized composite theory is based upon the premise that estimates of macroscopic properties can be recovered when local properties, and the details of their space-filling distribution, are known. [Recent work of Yoshida et al. (2003) proposes to work this problem in reverse—recovering local properties from macroscopic measurements.] A hierarchy of approximations derive from the theory such that, as increasing levels of microstructure detail are provided, more reliable estimates of macroscopic properties are achieved. Often these estimates are in terms of upper- and lower-bounds on properties; and increasing complexity in the microstructure hierarchy is rewarded with increasingly narrow bounds.

Generalized composite theory presumes that the physics that link the atomic-scale structure of a material point to the local properties of that point are known. For this reason, it can be considered to be a *mesoscale* theory. It has the considerable advantage, when dealing with polycrystalline materials, that its methodology makes close connections to the class of experimental methods commonly known as orientation imaging microscopy (OIM), and its union with energy dispersive spectroscopy (EDS) to obtain local determination of composition, crystal phase and lattice orientation. A concise review of the state-of-the-art in these methods has been presented in Schwartz et al. (2000).

The basic principle upon which MSD rests is that the intrinsic properties of a local material point are dependent upon a finite number of variables of local state; and these are presumed known to the observer. Primitive descriptors of local state include phase and composition. Additional parameters are important in crystalline materials, such as the crystal lattice orientation, hereafter referred to as *orientation*. (Orientation is the second-order tensor describing the rotation of a specified reference crystal to coincide with the local crystal orientation; Bunge, 1982; Adams and Olson, 1998). Orientation distribution is an important source of anisotropy in many properties. Other considerations, such as the defect-state, can be described, with varying degrees of completeness, by appending additional scalar and tensorial parameters to this basic set.

Note that microstructure-properties relations differ in their sensitivity to different components of the microstructure. For example, embrittlement is often a consequence of the local state of material points lying on (or near) the grain boundaries in crystalline materials, and has little dependence, if any, upon the state of material points lying in the grain interiors.¹ This can be contrasted with defect-insensitive properties, such as elasticity and thermal conductivity, that are primarily dependent upon the local state distribution in the grain interiors. Three basic kinds of knowledge are required to advance microstructure-property relations: (1) discernment of the (correct) components of microstructure in which the property resides; (2) enumeration of the particular local state variables and their associated property relations for the salient components; and (3) suitable homogenization relationships relating the spatial distribution of local properties to the effective (macroscopic) properties of interest. Since any microstructure design methodology that would require an exhaustive description of all aspects of the microstructure and the local state is known to lie well beyond our computational capacities for the foreseeable future, modeling of microstructure-properties relationships requires great care to select those attributes that most strongly impact effective properties.

It is useful to compare the linear methodology of this paper with the approach called 'topology optimization'. Topology optimization is focused on achieving extreme or unusual properties through control of the topology of the substructure. Most of the work thus far pertains to two-phase composites. Materials with negative thermal expansion, have been studied by Sigmund and Torquato (1996). Microstructures with negative Poisson's ratios have been studied and fabricated by Larsen et al. (1997). Elevated piezo-properties for applications in hydrophones have been studied by Sigmund et al. (1998). In these and other examples the topology of a composite substructure, consisting of components of widely varying properties (such as a mixture of solid and void phases), is essential to the recovery of remarkable properties. The problems addressed by topology optimization are

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¹ Grain boundaries or interfaces can be described, to a certain level of completeness, by consideration of the near-field two-point correlations of local state. Thus, the state of the boundary or interface is described by the correlation of local state variables across the boundary or interface.

inherently nonlinear in their dependence upon the descriptors of microstructure, and they require a suite of nonlinear optimization methods for their solution. Nonlinear problems also occur within the MSD framework described here; and their solution requires methods similar to those used in topology optimization (Henrie et al., 2002).

It is emphasized that the presentation of the spectral method described in this paper is based entirely upon first-order bounding principles for elastic and plastic properties, where these have linear dependence in the descriptors of microstructure. First-order bounds require only the volume-fraction distribution of components of the material, and therefore do not address anything about the spatial distribution of these phases, or their topology. However, we emphasize that the first-order bounds include all property combinations that are obtainable by varying topologies at constant volume-fraction distribution.

Throughout the paper, local mechanical properties are anticipated to depend only upon local crystal phase, phase orientation, and a single scalar state variable. It will be evident, by taking this path, how the work might be extended to more complex cases where additional scalar and/or tensorial variables of the local state are pertinent. In an effort to maintain simplicity, in the selected application we have restricted our attention to the specialized case of single-phase cubic materials possessing orthorhombic specimen symmetry, and where loading is parallel to the principal axes of the orthotropy. Orthotropy develops, typically, in rolled sheet and plate materials (cf. Rollett and Wright, 1998). The alloy system treated in more detail is isomorphous Cu–Ni, where the scalar state variable is conveniently identified with composition.

2. Representations of local state and properties

Assume that the microstructure components of interest have been identified through the physical evidence. Let h denote the local state at a material point: $h \in H$. H denotes the set (space) of all possible local states, and is called the *local state space*. It is assumed that local properties of interest, $p_1, p_2, \dots$, are known functions of the local state:

$$p_i = p_i(h). \quad (1)$$

Homogenization relations, described later, will be used to recover the associated macroscopic properties of interest, $P_1, P_2, \dots$, by considering these local properties and their distribution in the relevant microstructure component.

Consider, as an example, how the local state might be described at interior points in a crystalline material comprising two constituent phases (both crystalline). Suppose that the local state can be specified by its phase, ϕ , by the local lattice orientation of its phase, g , and by one additional scalar parameter, λ . λ may represent different characteristics in each phase. Thus, the local state at location x , $h(x)$, is given by the ordered set of parameters:

$$h(x) = \{\phi(x), g(x), \lambda(x)\}. \quad (2)$$

Each of the parameters of local state resides in a *fundamental set* or *fundamental zone*, depending upon whether the parameter belongs to a discrete set, or a continuous one. Phase belongs to a fundamental set consisting of, say, two elements, $\phi \in \{1, 2\} = \Phi$. Phase orientation belongs to one of two fundamental zones that are distinguished from each other by the distinctive symmetry subgroup of the phase; thus $g \in SO(3)/G_\phi = \Gamma_\phi$, where $SO(3)$ denotes the three-dimensional special orthogonal group of rotations and G_ϕ denotes the crystallographic symmetry subgroup of phase ϕ . $SO(3)/G_\phi$ is the orbit space of right G_ϕ cosets of $SO(3)$ (cf. Bröcker and tom Dieck, 1985), and hence represents the set of all physically-distinctive lattice orientations of phase ϕ . Finally, the scalar parameters associated with each phase are appropriately dilated and translated so as to be isomorphous with the unit interval on the real line, $\lambda \in [0, 1] = \Lambda$.

It is convenient, in view of relation (2), to consider a combined fundamental zone that represents the local state space H :

$$H = H_1 \bigcup H_2. \quad (3)$$

Here H_1 and H_2 are defined by the cartesian products

$$H_\phi = \Gamma_\phi \times \Lambda. \quad (4)$$

Local properties, of the form described in relation (1), are typically real-valued, square-integrable functions of the form $f: H \rightarrow \mathfrak{R}$. Such can be expressed as a weighted sum of orthonormal basis functions. Suitable basis functions for the relevant fundamental zones, Γ_1 , Γ_2 , and Λ are well known in the literature. For example, classical crystal-symmetric generalized spherical harmonic functions are used as a basis on Γ_ϕ (Bunge, 1982). Formally, these functions, ${}^\phi T_l^{\mu\nu}(g)$, are special linear combinations of the generalized spherical harmonic functions $[T_l^{mn}(g)$, cf. Gel'fand et al., 1963] according to the relation

$${}^\phi T_l^{\mu\nu}(g) = \sum_{m=-l}^l {}^\phi A_l^{m\mu} T_l^{mn}(g). \quad (5)$$

The symmetry coefficients, ${}^\phi A_l^{m\mu}$, depend upon the symmetry subgroup of the crystalline phase, G_ϕ (Bunge, 1982). Crystal symmetric functions have the property that

$${}^\phi T_l^{\mu\nu}(g_\phi \cdot g) = {}^\phi T_l^{\mu\nu}(g) \quad (6)$$

for any element of the symmetry subgroup of the crystalline phase.² Exponential functions provide a basis for Λ (cf. Kaplan, 1973); for example, the set E

$$E = \{\exp(2\pi m i \lambda) \mid \lambda \in \Lambda, -\infty \leq m \leq \infty\} \quad (7)$$

comprises the complete set of orthonormal basis functions on Λ .

² The form of relation (6) is consistent with the “passive” framework used by Bunge (1982). As such the argument of the function on the left hand side of the equation is understood in terms of the direction cosines of the orientation and the symmetry element $g_\phi \in G_\phi$.

Local property functions of the form described in relation (1) can then be described by the series:

$$p_j(h) = p_j(\phi, g, \lambda) = \sum_{l=0}^{\infty} \sum_{\mu=1}^{\phi M(l)} \sum_{n=-lm=-\infty}^l \sum_{m=-\infty}^{\infty} \phi p_{jl}^{\mu nm} \phi T_l^{\mu n}(g) \exp(2\pi i m \lambda), \quad (8)$$

where it is understood that $\phi M(l)$ enumerates the crystal symmetric subspaces associated with phase ϕ and the primary index l (see Bunge, 1982).

The classical basis functions used in relation (8) can be normalized to satisfy the following orthogonality relations:

$$\int_{\Gamma_{\phi}} \phi T_l^{\mu n}(g) \phi T_{l'}^{\mu' n'}(g) dg = \frac{1}{2l+1} \delta_{ll'} \delta_{\mu\mu'} \delta_{nn'}, \quad (9)$$

where $*$ denotes the complex conjugate, and dg is the invariant measure on Γ_{ϕ} . Also,

$$\int_{\Lambda} \exp(2\pi m i \lambda) \exp(-2\pi n i \lambda) d\lambda = 2\pi \delta_{mn}. \quad (10)$$

It follows that, when $p_j(h)$ is known, the coefficients $\phi p_{jl}^{\mu nm}$ can be calculated from the relation

$$\phi p_{jl}^{\mu nm} = \left(\frac{2l+1}{2\pi} \right) \cdot \int_{\Lambda} \int_{\Gamma_{\phi}} p_j(\phi, g, \lambda) \phi T_l^{\mu n*}(g) \exp(-2\pi m i \lambda) dg d\lambda. \quad (11)$$

The full set of products of functions, $\{\phi T_l^{\mu n}(g) \cdot \exp(2\pi m i \lambda)\}$, forms a complete, orthonormal set of basis functions, spanning all square-integrable functions of the form $f: H \rightarrow \Re$ (Courant and Hilbert, 1989). Hence, linear combinations of these comprise functions that reside in a vector space spanned by this set. This includes functions of the type illustrated by relation (8). In this context, *the coefficients $\phi p_{jl}^{\mu nm}$ are the coordinates of a point in this vector space, representing the property function $p_j(h)$.*

The integrated product of two functions lying in this vector space will be required in subsequent sections, and given the complexity of the state space H it is important to consider this carefully. Let $p(h)$ and $q(h)$ be two (real-valued) functions on H . Define their product, $\langle p, q \rangle$, to be

$$\langle p, q \rangle = \int_H p(h) \cdot q(h) dh. \quad (12)$$

In view of the nature of H , this integration must be considered to take the form

$$\langle p, q \rangle = \sum_{\phi=1}^2 \int_{\Gamma_{\phi}} \int_{\Lambda} p(\phi, g, \lambda) \cdot q(\phi, g, \lambda) d\lambda dg. \quad (13)$$

And when the series representation of $p(h)$ and $q(h)$ is introduced into relation (13), it follows from (9) and (10) that

$$\langle p, q \rangle = \sum_{\phi=1}^2 \sum_{l=1}^{\infty} \sum_{\mu=1}^{\phi M(l)} \sum_{n=-lm}^{+l} \sum_{m=-\infty}^{+\infty} \phi p_l^{\mu m} \phi \tilde{q}_l^{*\mu m}, \quad (14)$$

where

$$\phi \tilde{q}_l^{*\mu m} = \left(\frac{2\pi}{2l+1} \right) \phi q_l^{*\mu m}. \quad (15)$$

(Hereafter the application of the tilde $\sim$ over any particular coefficient shall mean a renormalization of that coefficient like that shown in (15).)

One particular function on H of central interest to this work is the Dirac delta function, $\delta(h - h_j)$, defined by the expression

$$\int_{H'} \delta(h - h_j) dh = \begin{cases} 1 & \text{if } h_j \in H' \\ 0 & \text{otherwise} \end{cases} \quad (16)$$

where (16) must hold for all $H' \subset H$. Expressed in terms of the classical basis functions, evaluation of relations (11), (16) indicates that

$$\delta(h - h_j) = \sum_{l=0}^{\infty} \sum_{\mu=1}^{\phi M(l)} \sum_{n=-lm}^l \sum_{m=-\infty}^{\infty} \phi \tilde{T}_l^{*\mu m}(g_j) \exp(-2\pi i m \lambda_j) \phi T_l^{\mu m}(g) \exp(2\pi i m \lambda). \quad (17)$$

This Dirac function can be interpreted to represent the local state h_j , and the coefficients $\phi \tilde{T}_l^{*\mu m}(g_j) \exp(-2\pi i m \lambda_j)$ are the coordinates of a point in the Fourier space representing local state h_j . Thus, an alternative description for the local state space H is the set of all coordinates of points in Fourier space, representing Dirac functions centered at all possible local states. Let H_f be this set, which is isomorphic to H ($H_f \leftrightarrow H$). Formally, it consists of the points x in Fourier space that satisfy the relation

$$H_f = \left\{ x = \{ \phi d_l^{\mu m} \} \mid \phi d_l^{\mu m} = \phi \tilde{T}_l^{*\mu m}(g) \exp(-2\pi i m \lambda), \forall (\phi, g, \lambda) \in H \right\}. \quad (18)$$

This is the *Fourier representation of the local state space* that will be of primary interest hereafter.

An alternative to the preceding classical representation of functions on H , based on a class of piecewise-constant functions, is available and can be used to advantage in some problems. The basic ideas are presented in the Appendix.

3. Elementary microstructure–property relations

The term *homogenization relationship* will refer here to any formal relationship between local properties, the microstructure, and macroscopic (effective)

properties. It is beyond the scope of this paper to derive the homogenization relations that are used; the position is taken that these are available for some important set of properties, and that they will be incorporated, as received, into the methodology for design of microstructure. A review of homogenization theories based in statistical continuum theory and with a focus on crystalline materials, was published by Adams and Olson (1998); the reader is referred to this and other primary works for more details. The aim here is to illustrate the typical form of these approximations, their explicit dependence upon microstructure, and their representation in Fourier space.

For the purposes of this paper, only elementary (first-order) homogenization theory is to be treated here. Elementary theory requires only volume-fraction information on the distribution of local states in the microstructure. Higher-order homogenization theories require, at a minimum, information about the two-point spatial correlations of local state variables. The extensions required for these are not treated in this paper. We note, however, that they are required for the description of defect-sensitive properties, as mentioned in the Introduction.

The term *microstructure representation* shall refer to the quantitative description of any specified part of the overall microstructure that is dictated to be of importance by the homogenization relation. When a combination of properties is important to the application, some attributes of microstructure may be important to one property, but not to another, within the physical framework of the homogenization relations. Few properties, however, are expected to be entirely independent of others, and there will generally be some overlapping between the components of the salient representations.

3.1. Elementary homogenization relations (elasticity)

First consider the problem of elasticity, where C^* denotes the fourth-order effective (macroscopic) stiffness tensor, $C = C(h)$ denotes the local stiffness at a material point, and ε is the second-order infinitesimal strain tensor. Let $\langle \dots \rangle$ denote the volume average of $(\dots)$. Application of the principle of minimum potential energy leads to elementary bounds on stored strain energy density (Hill, 1952; Paul, 1960):

$$\varepsilon_{ij} \langle S \rangle_{ijrs}^{-1} \varepsilon_{rs} \leq \varepsilon_{ij} C_{ijrs}^* \varepsilon_{rs} \leq \varepsilon_{ij} \langle C \rangle_{ijrs} \varepsilon_{rs}. \quad (19)$$

(Note that S is the fourth-order elastic compliance tensor, related to C by inversion.) Relation (19) is hereafter shortened to the form

$$\langle S \rangle_{ijrs}^{-1} \leq C_{ijrs}^* \leq \langle C \rangle_{ijrs}, \quad (20)$$

but it must always be remembered that the interpretation of (20) is in terms of the stored elastic energy.

For statistically homogeneous polycrystals, the right-hand (upper-bound) in relation (20) reduces to

$$C_{ijrs}^* \leq \langle C \rangle_{ijrs} = \int_H f(h) \cdot C_{ijrs}(h) dh = \langle f, C_{ijkl} \rangle, \quad (21)$$

where $f(h)$ is the (one-point) *local state distribution function*. $f(h)$ describes the volume fraction of the material that associates with local states in the vicinity, dh , of local state h , according to

$$\frac{dV}{V} = f(h)dh. \quad (22)$$

Note that both $f(h)$ and the components $C_{ijrs}(h)$ are real-valued functions on the local state space H . As such they admit spectral representations on either the classical [Eq. (8)] or the piecewise-constant basis (see Appendix). Let $\phi f_l^{\mu nm}$ denote the coefficients of $f(h)$, and $\phi C_l^{\mu nm}(ijrs)$ the coefficients of $C_{ijrs}(h)$ in the classical basis. Then relation (14) can be used to obtain the Fourier representation of the upper-bound on C^* :

$$C_{ijrs}^* \leq \langle f(h), C_{ijrs}(h) \rangle = \sum_{\phi=1}^2 \sum_{l=1}^{\infty} \sum_{\mu=1}^{\phi M(l)} \sum_{n=-lm=-\infty}^{+l} \sum_{m=-\infty}^{+\infty} \phi f_l^{\mu nm} \phi \tilde{C}_l^{*\mu nm}(ijrs). \quad (23)$$

In a development that exactly parallels the above, one obtains a Fourier representation for an upper bound on the effective compliance tensor, S^* :

$$S_{ijrs}^* \leq \langle f(h), S_{ijrs}(h) \rangle = \sum_{\phi=1}^2 \sum_{l=1}^{\infty} \sum_{\mu=1}^{\phi M(l)} \sum_{n=-lm=-\infty}^{+l} \sum_{m=-\infty}^{+\infty} \phi f_l^{\mu nm} \phi \tilde{S}_l^{*\mu nm}(ijrs). \quad (24)$$

Relation (24) is comprised of elements of a 6×6 matrix of compliance coefficients, that can be inverted using standard procedures (Hirth and Lothe, 1968) to obtain S^{*-1} . The lower-bound on the left hand side of relation (20) is just

$$S_{ijrs}^{*-1} \leq C_{ijrs}^*. \quad (25)$$

Whereas the upper-bound is linear in the coefficients of microstructure, $\phi f_l^{\mu nm}$, the lower-bound is clearly non-linear in these.

3.2. Elementary homogenization relations (initial plastic yielding)

In this section we briefly review two basic homogenization relationships for rate-insensitive plasticity. The first of these is attributed to Sachs (1928), and is not a bound on yielding, but is known to always lie inside the Taylor (1938) upper-bound on initial yielding, which is the second relation that will be described.

Consider first the Sachs model. The Cauchy stress, σ , in any crystallite of the composite material is assumed to be a simple scalar multiplier of a fixed unit stress $\hat{\sigma}$:

$$\sigma = \lambda \hat{\sigma} \quad (26)$$

In Sachs' model the unit stress is taken to be constant among all components of the material body. The scaling parameter is dependent upon the local state h in the crystallite, which is determined in a particular way. It is considered that plastic yielding occurs when the resolved shear stress on any particular slip system of the crystallite reaches a critical level (Schmid's law). For a crystallite of phase ϕ , and with slip system s , characterized by the unit slip plane normal $\phi \hat{n}^{(s)}$ and the unit slip

direction $\phi \hat{b}^{(s)}$, the resolved shear stress is $\phi \tau^{(s)} = \phi \hat{n}^{(s)} \lambda \hat{\sigma} \phi \hat{b}^{(s)}$. It is convenient to write this expression in terms of the fundamental slip tensor $\phi \mu^{(s)}$, as

$$\phi \tau^{(s)} = \phi \mu^{(s)} \lambda \hat{\sigma}, \quad (27)$$

where

$$\phi \mu_{ij}^{(s)} = \frac{1}{2} \left(\phi b_i^{(s)} \phi n_j^{(s)} + \phi b_j^{(s)} \phi n_i^{(s)} \right). \quad (28)$$

Next, let $\phi \tau_c^{(s)}$ denote the critical resolved shear stress at which slip on slip system s in phase ϕ occurs. This happens at different levels of the scaling parameter $\phi \lambda^{(s)}$ for each slip system. Hence the yielding criterion for slip on system s in phase ϕ is just

$$\phi \tau^{(s)} = \phi \tau_c^{(s)}. \quad (29)$$

According to Schmid (1926), yielding occurs at a given material point of local state h when the first slip system is activated upon loading. Thus, if s^* denotes the particular slip system that is first activated, then $\phi \lambda^{(s^*)}$ is the minimum among the scaling factors among available set of slip systems $\{\phi \lambda^{(s)}\}$. For convenience in notation we hereafter set the local stress estimate, $\sigma = \sigma(h)$, to be

$$\sigma(h) = \phi \lambda^{(s^*)} \hat{\sigma} = \lambda^* \hat{\sigma}, \quad (30)$$

where it is understood that $\lambda^* = \lambda^*(h, \hat{\sigma}) = \phi \lambda^{(s^*)}$ derives its dependence upon local state h through $\phi \tau_c^{(s)}$ and $\phi \mu^{(s)}$.

Sachs' model estimates the macroscopic stress, say $\bar{\sigma}$, to be the volume average of $\lambda^* \hat{\sigma}$:

$$\bar{\sigma} \approx \langle f, \lambda^* \rangle \hat{\sigma}, \quad (31)$$

where $f = f(h)$ is the local state distribution function described in (22). Now let the Fourier coefficients of the function λ^* be $\phi L_l^{unm}(\hat{\sigma})$. It follows from (14) that

$$\bar{\sigma}_{ij} \approx \sum_{\phi=1}^2 \sum_{l=1}^{\infty} \sum_{\mu=1}^{\phi M(l)} \sum_{n=-lm}^{+l} \sum_{m=-\infty}^{+\infty} \phi f_l^{unm} \phi \tilde{L}_l^{*unm}(\hat{\sigma}_{ij}). \quad (32)$$

Relation (32) is the representation of Sachs' estimate for initial plastic yielding, expressed in the Fourier space.

The second homogenization relationship for initial yielding is that of Taylor (1938), and is often called the *full constraints Taylor model*. It is also based upon the same idealization of crystallographic slip invoked in Sachs' model. Following Hill (1965), consider all possible displacement fields satisfying uniform-strain boundary conditions,

$$u_i = d\bar{e}_{ij} x_j \quad (\vec{x} \in \partial B), \quad (33)$$

where $d\bar{e}$ is a constant plastic strain-increment tensor, which also prescribes the macroscopic plastic strain, and $\vec{u}$ is the displacement vector at any point $\vec{x}$ lying on the boundary ∂B of the body B . Based upon the minimum principle of Hill, it is known that among all of the possible displacement fields satisfying (33), the true field is the one that minimizes the increment of plastic work, dw^p . Any other field, sat-

isfying the same boundary conditions will have a larger increment of plastic work. It follows that the simplest upper bound on the increment of plastic work can be obtained by selecting the local plastic strain increment, $d\epsilon$, to be equal to $d\bar{\epsilon}$ at every point in the body:

$$d\epsilon(\vec{x}) = d\bar{\epsilon}. \quad (34)$$

$d\epsilon$ can be expressed in terms of the slip strengths, $\phi d\gamma^{(s)}$, and the fundamental tensors, $\phi \mu^{(s)}$, via the relation

$$d\epsilon_{ij} = \sum_{s=1}^{\phi S} \phi d\gamma^{(s)} \phi \mu_{ij}^{(s)}, \quad (35)$$

where $1 \leq s \leq \phi S$ enumerates the slip systems associated with phase ϕ . Based upon the principle of minimum internal work, among all possible combinations of active slip systems that fulfill relations (34) and (35), Taylor postulates that the correct set is that which minimizes the local internal plastic work increment, which is related to the critical resolved shear stresses and the slip strengths by the expression:

$$dw^p = \sum_{s=1}^{\phi S} \phi \tau_c^{(s)\phi} d\gamma^{(s)}. \quad (36)$$

For an arbitrary $d\bar{\epsilon}$ and local state h , a minimum of five independent slip systems are required to satisfy (35). [In typical ductile crystal phases, the number of available combinations of five independent slip systems can be much larger than five, and therefore the principle of minimum internal work must be used to select the correct set(s).] It is evident dw^p is dependent upon local state h through $\phi \tau_c^{(s)}$ and $\phi \mu^{(s)}$; it is also dependent upon $d\bar{\epsilon}$. An upper-bound on the macroscopic plastic work increment, dW^p , obtains from the volume average of dw^p . More precisely,

$$dW^p \leq \langle f, dw^p \rangle. \quad (37)$$

Now let the Fourier coefficients of the function dw^p be $\phi W_l^{\mu nm}(d\bar{\epsilon})$. It follows from (14) that

$$dW^p \leq \sum_{\phi=1}^2 \sum_{l=1}^{\infty} \sum_{\mu=1}^{\phi M(l)} \sum_{n=-lm}^{+l} \sum_{m=-\infty}^{+\infty} \phi f_l^{\mu nm} \phi \tilde{W}_l^{*\mu nm}(d\bar{\epsilon}). \quad (38)$$

Since $\bar{\sigma} d\bar{\epsilon} = dW^p$, it follows that

$$\bar{\sigma}_{ij} = \frac{\partial(dW^p)}{\partial(d\bar{\epsilon}_{ij})} \leq \sum_{\phi=1}^2 \sum_{l=1}^{\infty} \sum_{\mu=1}^{\phi M(l)} \sum_{n=-lm}^{+l} \sum_{m=-\infty}^{+\infty} \phi f_l^{\mu nm} \left[\frac{\partial \phi \tilde{W}_l^{*\mu nm}}{\partial(d\bar{\epsilon}_{ij})} \right]. \quad (39)$$

Relation (39) is the representation of Taylor's upper-bound for initial plastic yielding, expressed in the Fourier space.

3.3. Property-bounding surfaces and estimates

Equations of the form illustrated in (23), (24), (39) define *closed half-spaces* (Rockafellar, 1970) in the spectral representation. These are delineated from the entire space by the *bounding hyperplane* that is defined in each relationship at the condition of equality. Materials possessing combinations of allowable microstructure coefficients, $\phi f_l^{\mu m}$ satisfying these equations, are predicted by the homogenization relationship to have properties (elastic or plastic) that do not exceed the pertinent effective property (left hand side of each equation). The lower-bound relationship, expressed by (24), (25), comprises a *property-bounding hypersurface* that is non-linear in the allowable microstructure coefficients. Sachs' estimate for initial yielding, embodied in relation (32) is not a bounding relationship, although it is known to lie within Taylor's upper-bound. It has the form of a hyperplane in the spectral representation, and all microstructures lying on a specified plane are estimated to have the same initial yield point.

4. The microstructure hull

Having specified bounding surfaces and estimates associated with the basic homogenization relationships, it is next essential to describe the set of all allowable microstructures. For the elementary homogenization relations described in this paper, all of the microstructures of interest belong to the set of all possible volume-fraction distributions on the local state space. This set is called the *microstructure hull*, Ω .

Any distribution on the local state space can be represented as the summation of a set of Dirac functions, weighted by appropriate volume fractions, v_j . All possible distribution functions thus belong to the set Ω :

$$\Omega = \left\{ f | f = \sum_j v_j \delta(h - h_j); \quad 0 \leq v_j \leq 1; \quad \sum_j v_j = 1 \right\}. \quad (40)$$

Note that the summation over j can be very extensive for weakly 'textured' materials. An alternative description resides in the Fourier space. Let the set Ω_f be isomorphic to Ω ($\Omega_f \leftrightarrow \Omega$). Ω_f consists of all points of coordinate sets $y = \{\phi f_l^{\mu m}\}$ in the Fourier space that satisfy the conditions

$$\Omega_f = \left\{ y | y = \sum_k v_k x_k; \quad x_k \in H_f; \quad 0 \leq v_k \leq 1; \quad \sum_k v_k = 1 \right\}, \quad (41)$$

where $x_k = \{\phi \tilde{T}_l^{* \mu m}(g_k) \exp(-2\pi m \lambda_k)\}$ according to relation (18).

The reader should note that the microstructure hull, Ω_f , is just the convex hull of the local state space H_f . Not only is it convex, but it is also compact; and these properties hold over any of its subspaces (Rockafellar, 1970).

5. Properties closures

The microstructures that are of interest to us are readily identified to be the intersection volume of the microstructure hull, Ω_f , with the pertinent bounding relationships and estimates [relations (23)–(25), (32), (39)]. It is typical, as will be illustrated in the application section of the paper, that properties bounding relationships and estimates are confined to finite dimensions in the Fourier space. Thus, beyond certain order in l (L) and m (Q), $\phi p_{jl}^{\mu m} \cong 0$. It follows from relation (14) that only those coefficients of the microstructure, $\phi f_l^{\mu m}$, that associate with $\phi p_{jl}^{\mu m} \neq 0$ affect the properties of interest. Thus, the focus of our interest lies in subspaces of the microstructure hull that associate with the properties of interest to the problem at hand.

When the pertinent properties bounds and estimates are linear in the coefficients of the microstructure, the set of all possible combinations of properties can be estimated through standard methods of linear analysis. The set of all possible combined properties, associated with a selected set of bounds or estimates is called a *properties closure*. The construction properties closures is considered next.

With reference to (18) and (41) define coefficients $\phi_k d_l^{\mu m}$ according to:

$$x_k = \{ \phi_k d_l^{\mu m} \} = \left\{ \phi T_l^{* \mu m}(g_k) \exp(-2\pi m \lambda_k) \right\}. \quad (42)$$

Properties relationships of the type exhibited in (23), (24), (32) and (39), which are linear in the coefficients of microstructure, can be written in the form

$$P_j \leq \langle f(h), p_j(h) \rangle = \sum_{\phi=1}^2 \sum_{l=1}^L \sum_{\mu=1}^{\phi M(l)} \sum_{n=-lm=-Q}^{+l} \sum_k^{+Q} v_k \phi_k d_l^{\mu m} \phi \tilde{p}_{jl}^{* \mu m}, \quad (43)$$

where k is summed over a selected basis set of Dirac functions spanning H_f , and L and Q indicate the finite levels of truncation of the series associated with the particular property of interest. Suppose we seek a properties closure for the set of properties $P_1 \rightarrow P_J$, where the set of integers $\{1, 2, \dots, J\}$ enumerate the properties of interest. To proceed, maximize or minimize P_1 for fixed $P_2, P_3, \dots, P_J$. This requires repeated solutions to the following standard problem in linear analysis:

$$\begin{aligned} \text{Maximize/Minimize } P_1 &= \sum_{\phi=1}^2 \sum_{l=1}^L \sum_{\mu=1}^{\phi M(l)} \sum_{n=-lm=-Q}^{+l} \sum_k^{+Q} v_k \phi_k d_l^{\mu m} \phi \tilde{p}_{1l}^{* \mu m} \\ \text{Subject to } P_2 &\leq \sum_{\phi=1}^2 \sum_{l=1}^L \sum_{\mu=1}^{\phi M(l)} \sum_{n=-lm=-Q}^{+l} \sum_k^{+Q} v_k \phi_k d_l^{\mu m} \phi \tilde{p}_{2l}^{* \mu m} \\ &\vdots \\ &\vdots \\ P_J &\leq \sum_{\phi=1}^2 \sum_{l=1}^L \sum_{\mu=1}^{\phi M(l)} \sum_{n=-lm=-Q}^{+l} \sum_k^{+Q} v_k \phi_k d_l^{\mu m} \phi \tilde{p}_{Jl}^{* \mu m} \\ v_1, v_2, \dots, v_K &\geq 0; \quad \sum_{k=1}^K v_k = 1 \end{aligned} \quad (44)$$

It is evident that the choice of property function to be maximized or minimized, from the set of combined properties of interest, is unimportant to the overall solution for the properties closure, as long as the closure is convex.³ Methods for solving systems of equations of the type described in (44) are well described in the literature, and are repeated here. For an introduction to the standard methods of solution the text of Strayer (1989) is recommended.

Although the application of standard methods of linear analysis is evidently applicable to the linear property functionals described in (23), (24), (32) and (39), the linear methodology can also be used to partially establish properties closures involving the lower-bound on elastic properties. It is known that the ‘extreme points’ associated with relation (44) consist of polystate microstructures where the number of components is equal to or less than the number of constraints in (44) (cf. Strayer, 1989, p. 16). Also for single state microstructures the upper- and lower-bounds coincide [as is evident from relations (16), (19)–(25)]. It follows that elastic property closures derived from upper- and lower-bounds will coincide over that set of extreme points that coincide single-state microstructures. For elastic properties closures it has been our experience (Henrie, 2002) that a substantial fraction of the properties closure derives from single-state microstructures, and therefore the differences in closures obtained via lower-bound homogenization relations are not very different from those obtained by the upper-bound relations for which relations (44) directly apply.

6. Application: elastic–plastic closures for single-phase cubic-orthorhombic materials

The main constructs of MSD are now illustrated for a simple class of materials. Our attention is focused on the isomorphous Cu–Ni alloy system, and upon microstructures within this system that exhibit orthorhombic sample symmetry. This material, across its entire range of composition, exhibits a face-centered-cubic structure possessing the point symmetry subgroup O_h .⁴ We shall denote this symmetry by setting $\phi = c$ in the equations that follow. The scalar state parameter λ will represent the composition of the alloy, in volume percent. We shall focus on applications that are suitably addressed with a lower-bound on the elastic compliance tensor, and with the Sachs estimate (pseudo-lower-bound) on the yield strength. In this case it is convenient to perform MSD in the Fourier space because the essential homogenization relationships are linear in the coefficients of microstructure.

³ Convexity of the microstructure hull does not require that the properties closures will also be convex. This requires a certain care in the application of relations (44) when non-convex closures are encountered.

⁴ Considerations of ordering that occur in this material at temperatures below 322 °C and Ni concentrations in the range of 33–97 wt.%, are not explicitly included in the present treatment, although the effects of such ordering are expected to have impact on some local properties relationships.

6.1. The local state distribution and the cubic-orthorhombic microstructure hull

Since the material of interest is single phase, the local state distribution function has the form $f(h) = f(g, \lambda)$. Orthorhombic sample symmetry is manifest in the local state distribution function by the following symmetry relations:

$$f(g, \lambda) = f(g \cdot \varphi, \lambda) \quad (\varphi \in D_2) \quad (45)$$

where D_2 is the orthorhombic symmetry subgroup. (D_2 comprises the identity element, and three two-fold rotations about the principal axes of the sample.) This symmetry reduces the number of basis functions in the spectral representation of the local state distribution function. Specifically, the cubic-orthorhombic (symmetrized) generalized spherical harmonic functions, named ${}^c\dot{T}_l^{\mu\nu}(g)$, have the property that ${}^c\dot{T}_l^{\mu\nu}(g \cdot \varphi) = {}^c\dot{T}_l^{\mu\nu}(g)$ for $\varphi \in D_2$, and ${}^c\dot{T}_l^{*\mu\nu}(g) = {}^c\dot{T}_l^{\mu\nu}(g)$ (Bunge, 1982).⁵ We shall represent the local state distribution function

$$f(h) = f(g, \lambda) \cong \sum_{l=0}^{\infty} \sum_{\mu=1}{{}^cM(l)} \sum_{\nu=1}{{}^cN(l)} \sum_{m=1}^Q {}^c f_l^{\mu\nu m} {}^c\dot{T}_l^{\mu\nu}(g) \vartheta_m(\lambda), \quad (46)$$

where the composition dependence of the problem is carried by the orthogonal piecewise-constant functions $\vartheta_m(\lambda)$ described in the Appendix, and ${}^cN(l)$ enumerates the sample-symmetric subspaces associated with orthorhombic sample symmetry (Bunge, 1982). (The reason for this choice is that the composition dependence of the elastic constants is nearly linear in λ , and it follows that high orders of the exponential functions would be required to obtain satisfactory approximations for the λ -dependence. For our purposes here, using the piecewise-constant basis, it will be sufficient to set $Q \approx 20$.) A typical 3-D subspace of the microstructure hull is shown in Fig. 1.

The upper-right index m^* indicates that a particular (homogeneous) composition is selected, associated with a composition that lies in $\vartheta_{m^*}(\lambda)$.

6.2. Elastic local property and homogenization relations in the cubic-orthorhombic Cu–Ni alloy system

Cubic crystal symmetry imparts the following orientation dependence to components of the elastic stiffness tensor:

$$C_{ijkl} = C_{12}^0 \delta_{ij} \delta_{kl} + C_{44}^0 (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + (C_{11}^0 - C_{12}^0 - 2C_{44}^0) \sum_{r=1}^3 g_{ri} g_{rj} g_{rk} g_{rl} \quad (47)$$

where C_{11}^0 , C_{12}^0 , and C_{44}^0 are the basic constants in $\langle 100 \rangle$ reference directions of the reference crystal. (The form of components of the elastic compliance tensor is

⁵ The notation used here is similar, but not exactly that of Bunge (1982), due to additional requirements of the MSD formulation. The single dot above the T denotes the orthorhombic sample symmetry, as it does in Bunge's notation.

Fig. 1. Cubic-orthorhombic microstructure hull in its $l=4, m=m^*$ subspace. (Note that the intercepts on the axes are ${}^c f_4^{11m^*} = -4.58, 6.87$, ${}^c f_4^{12m^*} = \pm 5.04$, ${}^c f_4^{13m^*} = \pm 4.65$.)

identical to relation (47) upon replacing the basic coefficients with the corresponding S_{11}^0 , S_{12}^0 , and S_{44}^0 .) Those C_{ijkl} of the form C_{iiij} do not possess orthorhombic symmetry, but all others do. Thus, for example, $C_{ijij}(g \cdot \varphi) = C_{ijij}(g)$ ($\varphi \in D_2$), as is readily apparent from relation (47). The composition dependence of the basic constants, to a good approximation, has been shown to be linear (Hartley, 2001):

$$C_{ij}^0(\lambda) = (1 - \lambda)C_{ij}^{0(Cu)} + \lambda C_{ij}^{0(Ni)} \quad (ij = 11, 12 \text{ or } 44). \quad (48)$$

Thus, the Fourier representation of C_{ijij} can be expressed as

$$C_{ijij} \cong \sum_{l=0}^4 \sum_{\mu=1}^{M(l)} \sum_{\nu=1}^{N(l)} \sum_{m=1}^Q {}^c C_l^{\mu\nu m}(ijij) {}^c \dot{T}_l^{\mu\nu}(g) \vartheta_m(\lambda), \quad (49)$$

where only four of the cubic-symmetric generalized spherical harmonics appear in the series: ${}^c \dot{T}_0^{11}(g)$, ${}^c \dot{T}_4^{11}(g)$, ${}^c \dot{T}_4^{12}(g)$ and ${}^c \dot{T}_4^{13}(g)$. That only the generalized spherical harmonic functions up to order four in the primary index l make their appearance in the elastic constants is a consequence of the fourth order tensorial nature of elasticity (Bunge, 1982; Bohlke, et al., 2003). Hence, the number of terms in the series is $4Q$. Also, the subspace of the microstructure hull shown in Fig. 1 is the relevant subspace for relation (49) for any choice of m .

Equivalent expressions for S_{ijkl} have the same form as (47)–(49) upon replacing the basic constants with S_{11}^0 , S_{12}^0 and S_{44}^0 . And from these a lower-bound on the (nine-parameter, cubic-orthorhombic) elastic stiffness tensor takes a form analogous to relation (20) for the elastic stiffness:

$$\langle S \rangle_{ijij}^{-1} \leq C_{ijij}^*, \quad (50)$$

where from (8)

$$\langle S \rangle_{ijij} = \sum_{l=0}^4 \sum_{\mu=1}^{cM(l)cN(l)} \sum_{v=1}^Q \sum_{m=1}^Q {}^c f_l^{\mu\nu m} {}^c \tilde{S}_l^{\mu\nu m}(ijij), \quad (51)$$

and

$${}^c \tilde{S}_l^{\mu\nu m}(ijij) = \frac{{}^c S_l^{\mu\nu m}(ijij)}{(2l+1)M(\lambda_m)}. \quad (52)$$

[Note that $M(\lambda_m)$ is the measure of set λ_m as described in relations (A4)–(A6).] Construction of the lower-bound, according to (50), (51) requires inverting a 6×6 matrix whose elements are functions of the $4Q$ microstructure coefficients ${}^c f_l^{\mu\nu m}$. Standard methods are described by Hirth and Lothe (1968). When fully implemented, the equality relation in (50), $\langle C \rangle_{ijij}^{-1} = S_{ijij}^*$, describes a curved hypersurface in the $4Q$ -dimensional subspace associated with elastic properties. This hypersurface separates the subspace of microstructures into two parts—with the relevant part satisfying relation (50).

For materials of homogeneous composition, only microstructure coefficients of the form ${}^c f_l^{\mu\nu m^*}$ ($\lambda \in \lambda_{m^*}$) are non-zero. Among the four basis functions that carry the orientation dependence of the microstructure we have ${}^c \dot{T}_0^{11}(g) = 1$. From relations (46), (A5) and the orthogonality of the basis functions, it is also evident that ${}^c f_0^{11m^*} = 1$. For fixed m^* (fixed composition) only three variable coefficients of the cubic-orthorhombic microstructure impact the upper-bound elastic properties— ${}^c f_4^{11m^*}$, ${}^c f_4^{12m^*}$ and ${}^c f_4^{13m^*}$. From these variables the component of the microstructure hull that pertains to cubic-orthorhombic elastic properties can be constructed via relation (41). Thus, the pertinent part of the hull is that rendered in Fig. 1.

A graphical depiction of relation (23) for the case $C_{1212}^* \leq \langle C_{1212} \rangle = 63$ GPa is shown in Fig. 2 for an alloy of pure Ni. The plane shown divides the cubic-orthorhombic microstructure hull into two parts, one of which satisfies the selected bounding relationship and the other which is excluded. As the bounding hyperplane is translated through the microstructure hull in the positive ${}^c f_4^{14m^*}$ direction, increasing bounds on C_{1212}^* are found. Relations (50), (51) produce a hyper-surface for the elastic lower-bound. Fig. 2 shows the bounding hypersurface for $C_{1111}^* \geq \langle S \rangle_{1111}^{-1} = 320$ GPa as it transects the microstructure hull. As $\langle S \rangle_{1111}^{-1}$ increases, the hypersurface moves along the negative ${}^c f_4^{12m^*}$ axis. The extrema of these hyperplanes and hypersurfaces are used to identify the property closures introduced in Section 5.

Implementation of relationship (44) to obtain the combined $C_{1111}^* - C_{1212}^*$ properties closure is illustrated in Fig. 3. This closure considers all possible alloys within the Cu–Ni system. The combination of constraints, represented by $C_{1111}^* \geq \langle S \rangle_{1111}^{-1} = 320$ GPa and $C_{1212}^* \leq \langle C_{1212} \rangle = 63$ GPa, is identified by the shaded region of the closure bounded by lines A and B in Fig. 4.

Once an region of feasible design has been identified, as in Fig. 4, the next task is to identify microstructures that achieve the desired performance. The first step is to

Fig. 2. Depiction of the intersection of the $C_{1212}^* \leq \langle C_{1212} \rangle = 63$ GPa and the $C_{1111}^* \geq \langle S \rangle_{1111}^{-1} = 320$ GPa bounding relations for pure Ni. The 'acceptable area', highlighted in yellow, associates with microstructures that satisfy both bounds.

Fig. 3. Property closure of C_{1111}^* vs. C_{1212}^* of the Cu-Ni alloy system.

locate the applicable bounding hyperplanes (hypersurfaces) within the microstructure hull, as in Fig. 2. Thus, the 'acceptable area' associated with the feasible region, consisting of allowable sets of ϕf_l^{unm} , is determined. It is evident from Fig. 3, that the region of feasible design is identified with the Ni-rich portion of the elastic closure.

Fig. 4. Property closure with design constraints added at A and B.

Choosing pure Ni as the alloy for further study, various selections can be made, within the 'acceptable area' of the microstructure hull. One of these is shown in terms of the inverse pole-figures of its orientation distribution function, in Fig. 5.

Fig. 5. Inverse pole-figures for one microstructure of Ni that satisfies both the $C_{1111}^* \geq 320$ GPa and $C_{1212}^* \leq 63$ GPa bounds.

Fig. 6. Variation of the critical resolved shear stress, τ_c , as a function of wt.% Ni.

6.3. Implementation of the Sachs estimate for initial yielding in the cubic-orthorhombic Cu–Ni alloy system

Section 3.2 describes the basic formulation of Sachs' estimate for initial yielding. The main elements of the model are contained in relations (29)–(32). The local state dependence of the model is contained in the critical-resolved shear stress, ${}^c\tau_c^{(s)}$, and the fundamental slip tensor, ${}^c\mu^{(s)}$. As it applies to the Cu–Ni alloy system, the former carries the composition dependence of yielding, and the latter the orientational dependence.

Fig. 7. Closure for the uniaxial yield stress (Sachs estimate, normalized to the critical resolved shear stress for Cu) versus C_{1111}^* (normalized to the reference elastic modulus in Cu, $C_{11}^{0(Cu)}$).

The functional dependence of the critical resolved shear stress is approximated from the known quadratic dependence of the yield and tensile stresses in the Cu–Ni system (Callister, 2000). The approximation is shown in Fig. 6, where it is indicated that the maximum value of $^c\tau_c^{(s)}$ occurs at ~ 60 wt.% Ni.

Coefficients for λ^* , $^cL_I^{umm}$, were computed for the Cu–Ni system, and introduced into the homogenization relationship (32) in order to evaluate the predicted initial plastic yield stress. This has been combined with the upper-bound relationship on C_{1111}^* expressed in relations (23), (49), and the constrained maximization algorithm described in relations (44), to obtain a closure on the combined uniaxial–axial yield stress and C_{1111}^* for the cubic-orthorhombic Cu–Ni alloy system. This closure is shown in Fig. 7.

7. Summary and discussion

Designers of complex mechanical components are often confronted with an array of design objectives and constraints. Satisfactory solutions to highly-constrained design problems often require consideration of the combinations of properties that occur in anisotropic materials. Anisotropy of material properties is associated with microstructure, and quantitative descriptions of microstructure, beyond the grain size, have rarely been available in conjunction with properties data bases (cf. Ashby, 1992). The present work aims to introduce microstructure as a design variable for those highly-constrained design problems where material properties are design limiting.

Properties closures describe the locus of possible combinations of properties that are predicted to be possible, given the freedom to manipulate material microstructure. Figs. 3 and 7 are examples of properties closures for combinations of two properties. They are quite remarkable for the range of properties combinations that are predicted to be available. From Fig. 3 it is evident that larger variations are predicted for the shear modulus ($\sim 300\%$) as compared with the elastic modulus ($\sim 40\%$) for alloys of a fixed composition. When composition is considered the range of possible variations is much larger, as expected. Consideration of combined elastic modulus with uniaxial yield strength (via Sachs estimate) shows variations of $\sim 75\%$ in the yield strength at fixed composition (and greater than 200% when composition is considered). Although the largest variations are expected to coincide with differences in extreme points, corresponding to single-state microstructures, it is also evident that substantial variations are possible among the more accessible poly-state microstructures.

These property closures have been derived from homogenization relations that are linear in their relationship to the Fourier coefficients that describe microstructure by its local state distribution function. It has been assumed that these homogenization relationships are valid, but it must be pointed out that comparisons between theory and experiment have been limited. Some comparisons of first-order predictions of elastic and plastic properties in textured materials under simple loading states are reviewed by Bunge (1982, pp. 294–350). A careful study of elastic properties, and

their correlation with first- and second-order homogenization theories has been presented by Beran et al. (1996). The work of Stout and Kocks (1998) on the yield surfaces of fcc materials is exemplary of some few studies that have been performed under varied stress states. Although these comparisons show promise, it is apparent from the paucity of published comparisons that additional study would be highly desirable.

The methodology, described in this paper, involves standard algorithms for systems of linear equations. It is amenable to the graphical interpretation shown in Figs. 1 and 2. Estimates and bounding relations are described as hyperplanes and hypersurfaces in a Fourier space that contains a subregion representing all possible microstructures. This subregion is named the microstructure hull, because it is compact and convex. Consideration of the possible intersections of the pertinent hyperplanes and hypersurfaces with the microstructure hull recover the properties closures that are the central theme of this paper. Although the examples shown combine only two properties, the methodology described for obtaining them [as expressed in relation (44)] is readily applied to higher-dimensional combinations. Additional examples of two-property closures for cubic-orthorhombic elasticity have been published by Henrie (2002).

Treatment in the Fourier space of Taylor plasticity has been described in detail by Bunge (1982) and Park et al. (1993) in cases where it is convenient to specify displacement boundary conditions. However, traction boundary conditions are much more common in mechanical design, and the formulation of Taylor's model in this environment is nonlinear and more complex. Recovery of yield loci from Taylor's model has been described in other works (cf. Bunge et al., 1980; Van Houtte et al., 1995; Van Houtte, 2001). Application of Taylor's model within the framework of MSD, for problems where the boundary conditions are of the traction type, is described in Henrie et al. (2002).

The elementary description of microstructure used in this paper is termed 'first-order' because it involves only the volume fraction of occurrence of the possible local states within the material. Higher-order descriptions of microstructure have been incorporated in some homogenization relations (cf. Torquato, 2001; Adams and Olson, 1998), and these lead to refinements in properties prediction. However, these have not yet been fully implemented within the MSD framework.

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Appendix. Piecewise-constant approximations

Consider a class of piecewise-constant functions (also called ‘box functions’, cf. Keener, 2000) to be used as an alternative to the classical basis for approximating various functions on the state space H . These are to be constructed in a particular way. Begin by partitioning of the fundamental zone Γ_ϕ into a set of sub-domains, $\{\phi_{\gamma_i} | i = 1, 2, \dots, N_{\Gamma_\phi}\}$, satisfying the following properties:

$$\phi_{\gamma_i} \cap \phi_{\gamma_j} = \emptyset \ (i \neq j), \quad \bigcup_{i=1}^{N_{\Gamma_\phi}} \phi_{\gamma_i} = \Gamma_\phi. \quad (\text{A1})$$

Here, $\emptyset$ denotes the empty or null set. Define characteristic functions $\phi_{\chi_i}(g)$ according to

$$\phi_{\chi_i}(g) = \begin{cases} \frac{1}{M(\phi_{\gamma_i})} & \text{if } g \in \phi_{\gamma_i} \\ 0 & \text{otherwise} \end{cases}, \quad (\text{A2})$$

where $M(\phi_{\gamma_i})$ is the (invariant) measure of the set ϕ_{γ_i} (cf. Gel’fand, et al., 1963; Bunge, 1982). It is defined as

$$M(\phi_{\gamma_i}) = \int_{\phi_{\gamma_i}} dg. \quad (\text{A3})$$

Similarly, partition the fundamental zone Λ into a set $\{\lambda_i | i = 1, 2, \dots, N_\Lambda\}$, satisfying relations analogous to those in (A1):

$$\lambda_i \cap \lambda_j = \emptyset \ (i \neq j), \quad \bigcup_{i=1}^{N_\Lambda} \lambda_i = \Lambda. \quad (\text{A4})$$

Furthermore, define characteristic functions, $\vartheta_i(\lambda)$, by analogy with relation (A2):

$$\vartheta_i(\lambda) = \begin{cases} \frac{1}{M(\lambda_i)} & \text{if } \lambda \in \lambda_i \\ 0 & \text{otherwise} \end{cases}, \quad (\text{A5})$$

where $M(\lambda_i)$ is the measure of the set λ_i , defined as

$$M(\lambda_i) = \int_{\lambda_i} d\lambda. \quad (\text{A6})$$

These characteristic functions satisfy orthogonality relations of the form

$$\int_{\Gamma_\phi} \phi_{\chi_i}(g) \cdot \phi_{\chi_j}(g) dg = \frac{\delta_{ij}}{M(\phi_{\gamma_i})}, \quad (\text{A7})$$

and

$$\int_{\Lambda} \vartheta_i(\lambda) \cdot \vartheta_j(\lambda) d\lambda = \frac{\delta_{ij}}{M(\lambda_i)}. \quad (\text{A8})$$

Using these definitions, real-valued functions on H can be approximated by the series

$$f(h) = f(\phi, g, \lambda) \cong \sum_{i=1}^{N_\Lambda} \sum_{j=1}^{N_{\Gamma_\phi}} \phi F_{ij} \phi \chi_j(g) \vartheta_i(\lambda). \quad (\text{A9})$$

It must be recognized that the quality of approximation represented in relation (A9) is entirely dependent upon the quality of partitioning the fundamental zones, and the sensitivity of the function over the selected elements of the partitioning. The coefficients of the approximation can be recovered by the expression

$$\begin{aligned} \phi F_{mn} &\cong \mathbf{M}(\phi \gamma_m) \mathbf{M}(\lambda_n) \int_{\Lambda} \int_{\Gamma_\phi} f(\phi, g, \lambda) \phi \chi_m(g) \vartheta_n(\lambda) \, \text{d}g \, \text{d}\lambda \\ &= \int_{\lambda_n} \int_{\phi \gamma_m} f(\phi, g, \lambda) \, \text{d}g \, \text{d}\lambda. \end{aligned} \quad (\text{A10})$$

The relationship between elements of the piecewise constant basis and the classical basis can be recovered by noting that

$$\phi \chi_r(g) \vartheta_s(\lambda) = \sum_{l=0}^{\infty} \sum_{\mu=1}^{\phi M(l)+l} \sum_{n=-lm=-\infty}^{+\infty} \phi X_{rl}^{\mu n} V_s^m \phi T_l^{\mu n}(g) \exp(2\pi i m \lambda), \quad (\text{A11})$$

where $\phi X_{rl}^{\mu n}$ are the coefficients of the characteristic function $\phi \chi_r(g)$ and V_s^m are the coefficients of the characteristic function $\vartheta_s(\lambda)$, expressed in terms of the classical basis functions. Introducing relations (11) and (A11) into (A10) we obtain the following relationship between the coefficients of the function $f(\phi, g, \lambda)$ in the piecewise constant basis, ϕF_{rs} , relative to the coefficients in the classical basis, $\phi f_l^{\mu n m}$:

$$\phi F_{rs} = \sum_{l=0}^{\infty} \sum_{\mu=1}^{\phi M(l)+l} \sum_{n=-lm=-\infty}^{+\infty} \phi Y_{rsl}^{\mu n m} \phi f_l^{\mu n m}, \quad (\text{A12})$$

where

$$\phi Y_{rsl}^{\mu n m} = \left(\frac{2\pi \mathbf{M}(\phi \gamma_r) \mathbf{M}(\lambda_s)}{2l+1} \right) \phi X_{rl}^{*\mu n} V_s^{*m}. \quad (\text{A13})$$

A relationship equivalent to Eq. (14) is readily obtained from Eqs. (A7)–(A9):

$$\langle p, q \rangle = \sum_{\phi=1}^2 \sum_{i=1}^{N_\Lambda} \sum_{j=1}^{N_{\Gamma_\phi}} \left(\frac{\phi p_{ij} \phi q_{ij}}{M(\lambda_i) M(\phi \gamma_j)} \right). \quad (\text{A14})$$

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