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Homogenization modeling of thin-layer-type microstructures

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ABSTRACT

The purpose of this paper is to introduce a homogenization method for the material behavior of two-phase composites characterized by a thin-layer-type microstructure. Such microstructures can be found for example in thermally-sprayed coating materials like WC/Fe in which the phase morphology takes the form of interpenetrating layers. The basic idea here is to idealize the thin-layered microstructure as a first-order laminate. Comparison of the methods with existing homogenization schemes as well as with the reference finite-element model for idealized composites demonstrates the advantage of the current approach for such microstructures. Further an extension of the approach to a variable interface orientation is presented. In the end the current method is compared to results based on FE-models of real micrographs.

1. Introduction

The modeling of the material behavior of composites is generally based on a model for the behavior of each constituent or phase of the composite together with one for the interaction of the phases. Traditionally, highly-idealized analytical and semi-analytical models were developed for this purpose with the help of volume-averaging or homogenization methods (e.g., Reuss, Voigt, Hashin–Shtrikmann, and so on), and are limited to linear thermoelasticity. More recently, methods for this purpose based on the assumption of scale-separation and the concept of representative volume element (RVE) have been developed and applied. These include the Mori–Tanaka method (e.g., Benveniste, 1987), the interpolative double inclusion model (e.g., Pierard et al., 2004), interaction direct derivative (IDD) method (Zheng and Du, 2001; Du and Zheng, 2002), self-consistent schemes such as the GSCS (Christensen and Lo, 1979) or higher-order bounds (Torquato and Lado, 1992). For a further overview and details see Nemat-Nasser and Hori (1993, 1999). Generally-speaking, these latter methods consist of two steps. In the first step, a local problem for a single inclusion is solved in order to obtain a model for the material behavior at the RVE-level. The prototype here is the approach of Eshelby (1957) for the case of an ellipsoidal elastic inclusion in an infinite matrix. The second step consists of averaging the RVE-fields to obtain those for the composite as a whole (e.g., Mercier and Molinari, 2009). As before, the focus here has been on linear thermoelasticity, also in order to exploit linearity in the mathematical formulation. For this case efficient methods are at hand, which are discussed, e.g., in Klusemann et al. (2012b). By analogy, extensions of these methods to the inelastic case are generally based on linearized incremental formulations (e.g., Ponte Castaneda and Suquet, 1998) pertaining mainly to metal inelasticity. The pioneer work of Sachs (1928) and Taylor (1938) can be seen as first homogenization methods for plasticity. The modification of the Sachs model by a static model (Zaoui, 1970) lead to a model which assumes that each constituent is subjected to the same stress which is equal to the macroscopic one which lead to a lower bound for the effective behavior. In the Taylor model uniform plastic strains are assumed which are equal to the macroscopic ones which lead to a upper bound. Dvorak (1992) proposed the so called transformation field analysis (TFA) in which the plastic strain fields were assumed to be phase-wise constant to calculate the effective behavior of inelastic composite materials (see also Dvorak et al., 1994a,b). As discussed by, e.g., Molinari et al. (1997), many of these approaches neglect the interactions between the phases, something which results in too stiff behavior. Because of this, models were developed which take phase interaction into account in some fashion (e.g., Molinari et al., 1987; Lebensohn and Tome, 1993). Michel and Suquet (2003, 2004) modified the transformation field analysis to account for spatially heterogeneous plastic strain fields resulting, e.g., from the interaction between the phases, which is named nonuniform transformation field analysis. They applied these methods mainly to composites with elastic–plastic phases. This method was studied further by several authors. For example, Roussette et al. (2009) applied it to elastic–viscoplastic constituents, and Fritzen and Böhlke (2011) analyzed the effect of different particle morphology in a metal-matrix composite with this method. Originally the nonuniform transformation field analysis was

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used in combination with a fast fourier transform (FFT) framework (Moulinec and Suquet, 1998). An implementation into the finite element framework is given by Fritzen and Böhlke (2010). Recently Agoras and Ponte Castañeda (2011) presented a generalization to multi-scale systems of the "variational linear comparison" method of Ponte Castañeda (1991) which allows the conversion from classical bounds or estimates for linear material behavior to nonlinear material behavior. A fully computational approach which is getting more popular in recent times is the use of FE^2 techniques (e.g., Smit et al., 1998; Miehe et al., 1999; Feyel, 2003). An overview about this topic was given by Geers et al. (2010).

In general the direct computation of the effective properties is based on an RVE which is the smallest unit of material, which fully describes the material behavior. The determination of the minimum RVE size is a non-trivial task. Drugan and Willis (1996) and Monetto and Drugan (2004, 2009) presented approaches to obtaining the minimum size by a non-local approach. Kanit et al. (2003) studied the necessary RVE size for random microstructure not only with respect to the wanted precision but also with the number of realization of a given microstructure volume.

If the RVE is very small or the characteristic size of the system approaches that of the microstructure, size effects can occur (e.g., Fülöp et al., 2006; Klusemann et al., 2012d), which are not accounted for at the macroscale. Furthermore, large spatial gradients at the macro-scale cannot be resolved by these methods and they are in general restricted to standard continuum mechanics theory. Full extension to second-order to incorporate size-effects of the underlying microstructure can be found by several authors (e.g., Kouznetsova et al., 2004; Bargmann et al., 2010; Klusemann, 2012a). Describing local deformation state of microstructured materials by extended continuum theories is done (e.g., Forest, 2008; Jänicke et al., 2009). In other cases, (e.g., Böhlke et al., 2008) texture related microstructural effects are accounted for by using orientation distribution functions and texture coefficients to predict the resulting anisotropy in sheet metals and the path-dependent mechanical properties. Houtte et al. (2005) presented an advanced Taylor-type statistical multi-grain model (ALAMEL) which accounts for the interactions between neighboring grains which is used to calculate the deformation texture in cubic metals.

The purpose of the current work is to present a homogenization approach for two-phase composites whose microstructure is characterized by being layer- or lamellar-like (laminate model). Such microstructures are present for example in thermally-sprayed coatings. The layered phase morphology arising here is determined among other things by the nature of the manufacturing process. The current homogenization strategy is based on the idealization of such microstructure as first-order laminate (e.g., Silhavy, 1997; Ortiz et al., 2000). This kind of idealization is used in the literature for different applications.

Ahzi et al. (1995) proposed a method to estimate the overall elastic properties of semi-crystalline polymers showing a layered structure. In Ahzi et al. (2007) three approaches are presented to determine the effective elastic properties of such structure by using a two-phase inclusion model with a crystalline lamella and amorphous domain connected over a planar interface as the local representative element of the polymer. Viscoplastic Taylor-type models have been used by, for example, Parks and Ahzi (1990); Ahzi et al. (1990) and Lee et al. (1995) for the prediction of texture evolution for a semi-crystalline polymeric material with a layered structure. In this context formulated Lee et al. (1993a,b) a rigid-viscoplastic inclusion model. van Dommelen et al. (2003) extended this model to an elasto-viscoplastic formulation which is used to determine the deformation and texture evolution of semi-crystalline polymers under loading. In Lee et al. (2002) bicrystal-based averaging schemes are presented for modeling the behavior of polycrystals for rigid viscoplasticity at large deformations. In this work the local homogenization is achieved by volume-averaging the bicrystal and considering the jump conditions at the planar interface between the two crystals assumed as occurring in a layered structure. Ortiz et al. (2000) used the idea of laminates for the description of the evolution of microstructures which show lamellar dislocation structures at large strains under monotonic loading. In this work the microstructure is idealized as first-order laminate. Furthermore models based on the idealization of first-order laminates are used for the transformation interface between, e.g., austenite and martensite in the realm of phase transformations (e.g., Kouznetsova et al., 2009). One main difference to most previously mentioned approaches is the used energy approach in this work.

The paper begins in Section 2 with a brief summary of the visco-plastic material model for each phase of the two-phase composite under consideration. The current approach as based on first-order laminate theory is introduced in Section 3. After investigating the behavior of this model with the help of simple deformation cases together with corresponding FE results for layered composites in Section 4, a comparison of results from the laminate model with analogous ones from selected existing homogenization models (e.g., Taylor, phase-wise constant plastic deformation) is given in Section 5. Followed by a discussion of a variable interface direction in Section 6. Next in Section 7 the creation of FE-models based on real micrographs and comparison to the current homogenization approach are discussed. The work ends (Section 8) with a summary and conclusions. For simplicity, the current work is restricted to small deformation.

2. Material model

In the current work, material models are formulated in the context of continuum thermodynamics. In this context, the material behavior is related to energetic and dissipative processes. As usual, the energetic part is determined by the free energy density ψ. For simplicity, attention is restricted here to quasi-static conditions and metallic materials exhibiting small deformation and Voce (i.e., saturation) isotropic hardening. In this case, the additive form

$$\psi(\boldsymbol{E}_\mathrm{E}, \alpha_\mathrm{P}) = \frac{1}{2}\boldsymbol{E}_\mathrm{E}\cdot\mathcal{C}_\mathrm{E}\boldsymbol{E}_\mathrm{E} + s_\mathrm{H}\left\{\alpha_\mathrm{P} + \frac{1}{c_\mathrm{H}}(e^{-c_\mathrm{H}\alpha_\mathrm{P}} - 1)\right\} \tag{1}$$

of ψ into elastic and hardening contributions, respectively, is assumed. In particular, the former depends on the elastic strain

$$\boldsymbol{E}_\mathrm{E} = \boldsymbol{E} - \boldsymbol{E}_\mathrm{P}, \tag{2}$$

corresponding inelastic strain $\boldsymbol{E}_\mathrm{P}$, and total (small) strain $\boldsymbol{E} = \mathrm{sym}(\boldsymbol{F} - \boldsymbol{I})$, with $\boldsymbol{F}$ the deformation gradient. Here, $\mathrm{sym}(\boldsymbol{A}) := \frac{1}{2}(\boldsymbol{A} + \boldsymbol{A}^\mathrm{T})$, represents the symmetric part of any second-order tensor $\boldsymbol{A}$. The evolution of $\boldsymbol{E}_\mathrm{P}$ depends on that of the accumulated equivalent inelastic deformation α_P, as shown in (6) below. Material properties here include the elastic stiffness tensor $\mathcal{C}_\mathrm{E}$, the difference s_H between the initial and saturated values of the yield stress, and the rate c_H of hardening saturation. As usual, the free energy determines in particular the stress

$$\boldsymbol{T} = \partial_{\boldsymbol{E}_\mathrm{E}}\psi. \tag{3}$$

Assuming dislocation glide as the dominant mechanism of inelastic deformation, the inelastic behavior is determined by an inelastic potential ϕ_P modeled by the simple viscoplastic form

$$\phi_\mathrm{P}(\varsigma_\mathrm{P}) = \sigma_\mathrm{D}\dot{\alpha}_\mathrm{r}\left\{\exp\left(\frac{\langle\varsigma_\mathrm{P} - \sigma_\mathrm{A}\rangle_+}{\sigma_\mathrm{D}}\right) - \frac{\langle\varsigma_\mathrm{P} - \sigma_\mathrm{A}\rangle_+}{\sigma_\mathrm{D}}\right\} \tag{4}$$

for the activation of dislocation motion and inelastic deformation. Here, $\langle f\rangle_+ := \frac{1}{2}(f + |f|)$ represents the ramp function. In particular, this potential determines the flow rule

$$\dot{\alpha}_\mathrm{P} = \partial_{\langle\varsigma_\mathrm{P} - \sigma_\mathrm{A}\rangle_+}\phi_\mathrm{P} \tag{5}$$