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Modelling of planar interface elastic behaviour: Application to grain boundaries in polycrystals

Modélisation du comportement élastique d'interfaces planes : Application aux joints de grain dans les polycrystaux

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ABSTRACT

In polycrystalline elastic simulations, grain boundaries can be considered as volume interphases or as elastic interfaces assuming a displacement jump across the interface. Such an interface description does not account for the in-plane deformation of the interface and Poisson effects cannot be reproduced. The purpose of this Note is to provide an enriched description of the elastic interface which takes into account such effects. When considering a multilayer material, the interphase description and the enriched interface description yield identical homogenized behaviour while quite important discrepancies can be observed with the classical interface description.

RÉSUMÉ

Afin de réaliser des simulations du comportement élastique de polycristaux, les joints de grains peuvent être considérés comme des interphases volumiques ou comme des interfaces auxquelles on associe classiquement un saut de déplacement. Cette description ne prend pas en compte la déformation dans le plan de l'interface et ne peut rendre compte d'effets de type Poisson. L'objet de cette Note est donc de proposer une description enrichie du comportement élastique d'interfaces. Appliquées au cas d'un matériau multi-couches, les descriptions « interface enrichie » et « interphase volumique » conduisent à un comportement homogénéisé identique tandis que d'importants écarts sont observés avec la description « interface classique ».

1. Introduction

A polycrystal can be considered as an assembly of grains separated by grain boundaries, each grain being characterized by its crystallographic orientation. From an atomistic point of view, a grain boundary is characterized by a region of thickness h in which the atoms positions are not exactly situated on the ideal crystallographic positions of the two neighbouring grains. This discrepancy between the ideal positions and the real ones is due to the atom interactions and the exact position of atoms in grain boundaries can be obtained from empirical interatomic interaction simulations by relaxation of an initial configuration where the atoms are situated on their ideal positions (Refs. [1] and [2] are two examples among an abundant

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literature). The consequences arising from the relaxed configuration of the grain boundary are twice. First, intrinsic stresses and strains appear on the unloaded configuration and secondly, the elastic (and thermal) properties evolve across the thickness of the grain boundary and can be very different from the behaviour of the neighbouring grains [1,3–5]. This Note focuses on the last point and intrinsic stresses and strains are not considered.

To take into account the grain boundaries in continuum mechanics, two different approaches can be used. The first one is associated to an "interphase" description of the grain boundary: the grain boundary is considered as a new phase with varying or homogeneous elastic properties [6]. The second one is associated to an "interface" description: the grain boundary is considered as a surface associated to an interface elastic behaviour [5,7,8].

When considering the interface description in polycrystalline simulations, the interface elastic behaviour accounts for a displacement jump across the interface [5,7,8] and relates it to the normal stress applied to the interface. As the in-plane interface strain is not considered, different effects are neglected such as Poisson effects (i.e. when loading the interface with a uniaxial normal stress, the interface does not stretch). This description is referred as the "simplified" description.

The purpose of this Note is to provide an "enriched" description of the interface behaviour which takes into account Poisson effects. Moreover, a procedure to derive the interface elastic properties from the interphase description is proposed. Finally, calculations are performed on a multilayer material for which the exact homogenized elastic tensor can be obtained. The interphase description and the enriched interface description yield identical homogenized behaviour while quite important discrepancies can be observed with the "simplified" interface description.

Note that the behaviour of imperfect interfaces has been extensively studied by Hashin [9] and recently, in the continuity of Hashin, by Benveniste [10]. The following model, established for planar interfaces, can be regarded as an alternative model, which could be easily implemented in a finite element code, between the "simplified" model and their much more complex model. Finally, the comparison with Benveniste and Hashin's work is not straightforward and our approach can be considered as a new approach mainly based on the introduction of the so-called "localized" in-plane stress.

2. Interface elastic behaviour

2.1. Notations

The projections of stresses and strains in the plane (P) and out of the plane (A, for anti-plane) of the interface are often used in this section. Eq. (1) gives an example for an interface perpendicular to $\underline{e_1}$:

$$\underline{\underline{X}} = \underline{\underline{X^A}} + \underline{\underline{X^P}} \quad \text{with } \underline{\underline{X^A}} = \begin{pmatrix} X_{11} & X_{12} & X_{13} \\ X_{21} & 0 & 0 \\ X_{31} & 0 & 0 \end{pmatrix} \quad \text{and} \quad \underline{\underline{X^P}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & X_{22} & X_{23} \\ 0 & X_{32} & X_{33} \end{pmatrix} \tag{1}$$

A fourth order tensor T can be written with the same notations through the introduction of the four tensors T^{AP}, T^{PA}, T^{AA} and T^{PP} (Eq. (2)).

$$\underline{\underline{Y}} = T : \underline{\underline{X}} \quad \Leftrightarrow \quad \left\{ \begin{array}{l} \underline{\underline{Y^A}} = T^{AA} : \underline{\underline{X^A}} + T^{AP} : \underline{\underline{X^P}} \\ \underline{\underline{Y^P}} = T^{PA} : \underline{\underline{X^A}} + T^{PP} : \underline{\underline{X^P}} \end{array} \right\} \quad \Leftrightarrow \quad \left[\begin{array}{c} \underline{\underline{Y^A}} \\ \underline{\underline{Y^P}} \end{array} \right] = \left[\begin{array}{cc} T^{AA} & T^{AP} \\ T^{PA} & T^{PP} \end{array} \right] : \left[\begin{array}{c} \underline{\underline{X^A}} \\ \underline{\underline{X^P}} \end{array} \right] \tag{2}$$

For symmetric tensors $\underline{\underline{X}}$ and $\underline{\underline{Y}}$, T^{AP} can be written with a matrix notation $\tilde{T}^{AP}$ (Eq. (3)) and contains 9 parameters or 6 parameters if T^{AP} is symmetric. Notations T^{PA}, T^{AA} and T^{PP} follow the same description.

$$\begin{bmatrix} Y_{11} \\ \sqrt{2}Y_{12} \\ \sqrt{2}Y_{13} \end{bmatrix} = \left[\tilde{T}^{AP}\right] \begin{bmatrix} X_{22} \\ X_{33} \\ \sqrt{2}X_{23} \end{bmatrix} \tag{3}$$

2.2. Thermodynamic definition

To define the elastic behaviour of the interface, the first step consists in defining the kinematic and the stresses associated to an interface. We assume classically that a displacement jump $[\underline{u}]$ occurs between the two sides of the interface. In addition, the in-plane deformation $\underline{\underline{\varepsilon^P}}$, which is assumed to be constant across the interface, is considered. On the other hand, if the normal stress (i.e. $\underline{\underline{\sigma^A}}$) is assumed to be constant across the interface, the in-plane stress can be different from on side to another. To account for this jump, a "localized" in-plane stress, $\underline{\underline{\sigma^{P^*}}}$ (with the unit $\mathrm{N\,m^{-1}}$), is defined. As a consequence, the stresses and strains within a volume Ω with an interface S are given by Eqs. (4) and (5), where $\delta(S)$ is the Dirac function localized on the surface S, $\underline{\underline{\sigma^0}}$ and $\underline{\underline{\varepsilon^0}}$ the stresses and strains within the bulk part of the volume element. The surface density of internal power is given for the interface by Eq. (6):

$$\underline{\underline{\varepsilon}}(x) = \underline{\underline{\varepsilon^0}}(x) + \left([\underline{u}] \otimes^S \underline{n}\right)\delta(S) \tag{4}$$

$$\underline{\underline{\sigma}}(x) = \underline{\underline{\sigma^0}}(x) + \underline{\underline{\sigma^{P^*}}}\delta(S) \tag{5}$$

$$p_i = \underline{\underline{\sigma^A}} : \left([\underline{\dot{u}}] \otimes^S \underline{n}\right) + \underline{\underline{\sigma^{P^*}}} : \underline{\underline{\dot{\varepsilon}^P}} \tag{6}$$

To define the linear elastic behaviour of the interface, the surface density of free energy is given by a quadratic function of the state variables $[\underline{u}]$ and $\underline{\underline{\varepsilon}}^P$ (Eq. (7)), where C^{AA}, C^{PP}, C^{AP} and C^{PA} are fourth order tensors, with $C^{AP} = (C^{PA})^t$ and C^{AA} and C^{PP} symmetric tensors:

$$\psi\left([\underline{u}], \underline{\underline{\varepsilon}}^P\right) = \frac{1}{2}\left([\underline{u}] \otimes^S \underline{n}\right) : C^{AA} : \left([\underline{u}] \otimes^S \underline{n}\right) + \frac{1}{2}\underline{\underline{\varepsilon}}^P : C^{PP} : \underline{\underline{\varepsilon}}^P + \frac{1}{2}\left([\underline{u}] \otimes^S \underline{n}\right) : C^{AP} : \underline{\underline{\varepsilon}}^P + \frac{1}{2}\underline{\underline{\varepsilon}}^P : C^{PA} : \left([\underline{u}] \otimes^S \underline{n}\right) \tag{7}$$

From the Clausius–Duhem inequality (i.e. equality for the considered reversible behaviour) and the derivation of the surface density of free energy, the following relations can be derived for the elastic interface behaviour (Eqs. (8) and (9)). These relations can be written using a matrix notation (Eq. (10)), in which $\underline{e_1}$ is perpendicular to the interface direction:

$$\underline{\underline{\sigma}}^A = C^{AA} : \left([\underline{u}] \otimes^S \underline{n}\right) + C^{AP} : \underline{\underline{\varepsilon}}^P \tag{8}$$

$$\underline{\underline{\sigma}}^{P^*} = C^{PP} : \underline{\underline{\varepsilon}}^P + C^{PA} : \left([\underline{u}] \otimes^S \underline{n}\right) \tag{9}$$

$$\begin{bmatrix} \sigma_{11} \\ \sqrt{2}\sigma_{12} \\ \sqrt{2}\sigma_{13} \\ \sigma_{22}^{P^*} \\ \sigma_{33}^{P^*} \\ \sqrt{2}\sigma_{23}^{P^*} \end{bmatrix} = \left[\begin{array}{c:c} \tilde{C}^{AA} & \tilde{C}^{AP} \\ \hdashline \tilde{C}^{PA} & \tilde{C}^{PP} \end{array}\right] \begin{bmatrix} [u_1] \\ \sqrt{2}[u_2] \\ \sqrt{2}[u_3] \\ \varepsilon_{22}^P \\ \varepsilon_{33}^P \\ \sqrt{2}\varepsilon_{23}^P \end{bmatrix} \tag{10}$$

The classical interface elastic behaviour taken into account in polycrystalline simulations, analytically [7] or numerically [8], only considers the displacement jump across the interface and the elastic behaviour reduces to Eq. (11):

$$\begin{bmatrix} \sigma_{11} \\ \sqrt{2}\sigma_{12} \\ \sqrt{2}\sigma_{13} \end{bmatrix} = \left[\tilde{C}^{AA}\right] \begin{bmatrix} [u_1] \\ \sqrt{2}[u_2] \\ \sqrt{2}[u_3] \end{bmatrix} \tag{11}$$

2.3. From interphase behaviour to interface behaviour

As demonstrated from Molecular Dynamics calculations [4], a grain boundary can be considered as an interphase defined as a region of thickness h in which the elastic properties evolve continuously from the bulk properties of one grain to the bulk properties of the other grain. However, although continuous this evolution is not monotonous and the elastic properties within the interphase can be very anisotropic, and very different from the behaviour of the two neighbouring grains. Let us now consider a bimaterial as an infinite volume Ω with a planar interphase located at $x = 0$, and a macroscopic loading applied on the boundary of the infinite volume. The average stress and strain over Ω are respectively $\overline{\underline{\underline{\sigma}}}$ and $\overline{\underline{\underline{\varepsilon}}}$. Considering perfect interfaces between the interphase and the two materials, the normal stress and the in-plane strain within the interphase are equal to the average ones (Eq. (12)). The elastic behaviour of the interphase (Eq. (13)), that depends on x between $-h/2$ and $h/2$, can be written using Eq. (12):

$$\underline{\underline{\varepsilon}}^P(x) = \overline{\underline{\underline{\varepsilon}}}^P, \qquad \underline{\underline{\sigma}}^A(x) = \overline{\underline{\underline{\sigma}}}^A \tag{12}$$

$$\begin{bmatrix} \overline{\underline{\underline{\sigma}}}^A \\ \underline{\underline{\sigma}}^P(x) \end{bmatrix} = \begin{bmatrix} K^{AA}(x) & K^{AP}(x) \\ K^{PA}(x) & K^{PP}(x) \end{bmatrix} \begin{bmatrix} \underline{\underline{\varepsilon}}^A(x) \\ \overline{\underline{\underline{\varepsilon}}}^P \end{bmatrix} \tag{13}$$

This relation is partially inversed to obtain Eq. (14) and integrated over the interface thickness to provide Eq. (16). The integration of $\underline{\underline{\varepsilon}}^A(x)$ on the interphase thickness is related to the relative displacement of the two sides of the grain boundary ($[\underline{u}]$) (Eq. (15)) which can be regarded as the displacement jump across the interface as described in the previous section. The integration of $\underline{\underline{\sigma}}^P(x)$ on the interphase thickness ($\underline{\underline{\sigma}}^{P^*}$) can be regarded as the "localized" plane stress introduced previously. Finally, a partial inversion of Eq. (16) leads to Eq. (17) which corresponds to Eqs. (8) and (9). As a consequence, the interface elastic properties defined in the previous section can directly be derived from the evolution of the volume elastic properties within the interphase.

$$\begin{bmatrix} \underline{\underline{\varepsilon}}^A(x) \\ \underline{\underline{\sigma}}^P(x) \end{bmatrix} = \begin{bmatrix} T^{AA}(x) & T^{AP}(x) \\ T^{PA}(x) & T^{PP}(x) \end{bmatrix} \begin{bmatrix} \overline{\underline{\underline{\sigma}}}^A \\ \overline{\underline{\underline{\varepsilon}}}^P \end{bmatrix} \tag{14}$$

$$\int_{-h/2}^{h/2} \underline{\underline{\varepsilon}}^A(x)\,\mathrm{d}x = [\underline{u}] \otimes^s \underline{n} \tag{15}$$

$$\begin{bmatrix} [\underline{u}] \otimes^S \underline{n} \\ \underline{\underline{\sigma}}^{P^*} \end{bmatrix} = \begin{bmatrix} T^{AA^*} & T^{AP^*} \\ T^{PA^*} & T^{PP^*} \end{bmatrix} \begin{bmatrix} \underline{\underline{\overline{\sigma}}}^{A} \\ \underline{\underline{\overline{\varepsilon}}}^{P} \end{bmatrix} \tag{16}$$

$$\begin{bmatrix} \underline{\underline{\overline{\sigma}}}^{A} \\ \underline{\underline{\sigma}}^{P^*} \end{bmatrix} = \begin{bmatrix} C^{AA} & C^{AP} \\ C^{PA} & C^{PP} \end{bmatrix} \begin{bmatrix} [\underline{u}] \otimes^S \underline{n} \\ \underline{\underline{\overline{\varepsilon}}}^{P} \end{bmatrix} \tag{17}$$

The equations to obtain T^{IJ} from K^{MN} and C^{IJ} from T^{MN^*} are not detailed here. They involve elementary tensor manipulations and can be found in [11,12].

3. Application to a multilayer material

The purpose of this section is to evaluate, on a very simple example, the difference observed on the homogenized behaviour of a multilayer material using for the grain boundaries either an interphase description or the "classical" interface description (Eq. (11)) or the "enriched" description (Eq. (10)). The case of the multi-layer material is interesting because its homogenized behaviour can be derived without any approximation [11,12]. The material consists of homogeneous grain layers of thickness $d - h$ separated by homogeneous grain boundaries of thickness h.

In the case of an interphase description, the grain boundaries are considered as bulk layers. The stresses and strains within the bulk layers (the interphase layers and the grain layers) are homogeneous and satisfy Eqs. (12) and (14) (considering a homogeneous elastic behaviour in this case). The average stresses and strains are given by Eqs. (18) and (19). With this set of equations (Eqs. (12), (14), (18), (19)), the homogenized elastic tensor K^{h0} (so that $\underline{\underline{\overline{\sigma}}} = K^{h0} : \underline{\underline{\overline{\varepsilon}}}$) can be easily derived [11,12].

$$\underline{\underline{\overline{\varepsilon}}} = \left(1 - \frac{h}{d}\right) \underline{\underline{\varepsilon}}^{g} + \frac{h}{d} \underline{\underline{\varepsilon}}^{i} \tag{18}$$

$$\underline{\underline{\overline{\sigma}}} = \left(1 - \frac{h}{d}\right) \underline{\underline{\sigma}}^{g} + \frac{h}{d} \underline{\underline{\sigma}}^{i} \tag{19}$$

In the case of an interface description, the first step consists to derive the interface properties from the interphase behaviour (Eqs. (14) to (17)). Then, the stresses and strains within the grain layers are homogeneous and satisfy Eqs. (12) and (14). The stresses and strains (in a general sense) within the interface are homogeneous along the interface and satisfy Eq. (17). Assuming a zero-thickness interface, the average stresses and strains can be derived from Eqs. (4) and (5) (Eqs. (20a), (21a)). In order to account for the interphase thickness, the contributions of the grains are balanced by their volume fraction (Eqs. (20b), (21b)):

$$\underline{\underline{\overline{\varepsilon}}} = \frac{1}{V} \int_V \underline{\underline{\varepsilon}}(x)\, \mathrm{d}V = \underline{\underline{\varepsilon}}^{g} + \frac{1}{d} \left([\underline{u}] \otimes^S \underline{n} \right) \tag{20a}$$

$$\underline{\underline{\overline{\varepsilon}}} = \left(1 - \frac{h}{d}\right) \underline{\underline{\varepsilon}}^{g} + \frac{1}{d} \left([\underline{u}] \otimes^S \underline{n} \right) \tag{20b}$$

$$\underline{\underline{\overline{\sigma}}} = \int_V \underline{\underline{\sigma}}(x)\, \mathrm{d}V = \underline{\underline{\sigma}}^{g} + \frac{1}{d} \underline{\underline{\sigma}}^{P^*} \tag{21a}$$

$$\underline{\underline{\overline{\sigma}}} = \left(1 - \frac{h}{d}\right) \underline{\underline{\sigma}}^{g} + \frac{1}{d} \underline{\underline{\sigma}}^{P^*} \tag{21b}$$

From this set of equations (Eqs. (12), (14), (17), (20b), (21b)) the homogenized elastic tensor K^{h1} derived from the "enriched" interface description is identical to the exact solution K^{h0} while the tensor K^{h2} derived from the "simplified" interface description (using Eq. (11) instead of Eq. (17)) is different and then considered as an approximation.

For numerical application, the grain layers and the interphase are isotropic. The Young modulus of the interphase evolves between 10 and 1000 GPa whereas it is 100 GPa for the grain layers. Poisson coefficients are 0.1 for the grains and 0.4 for the interphases. The interphase thickness is 1 nm and the grain size d is 10 nm. The interphases are parallel to the $(\underline{e_2}, \underline{e_3})$ plane. The evolution of the five independent coefficients of the transverse isotropic tensors is displayed in Fig. 1 as a function of the interphase Young modulus. First, it can be observed that K_{11} and K_{55} (coefficient between σ_{13} and ε_{13}, and σ_{12} and ε_{12}) are not affected by the simplified description. Secondly, the difference between the exact solution and the approximated one (i.e. with the simplified interface description) can be very important on the other coefficients and increases when the stiffness of the interphase increases. Of course, this conclusion is limited to a specific set of isotropic behaviours for both the grains and the interphase and a detailed study has to be performed for anisotropic behaviours.

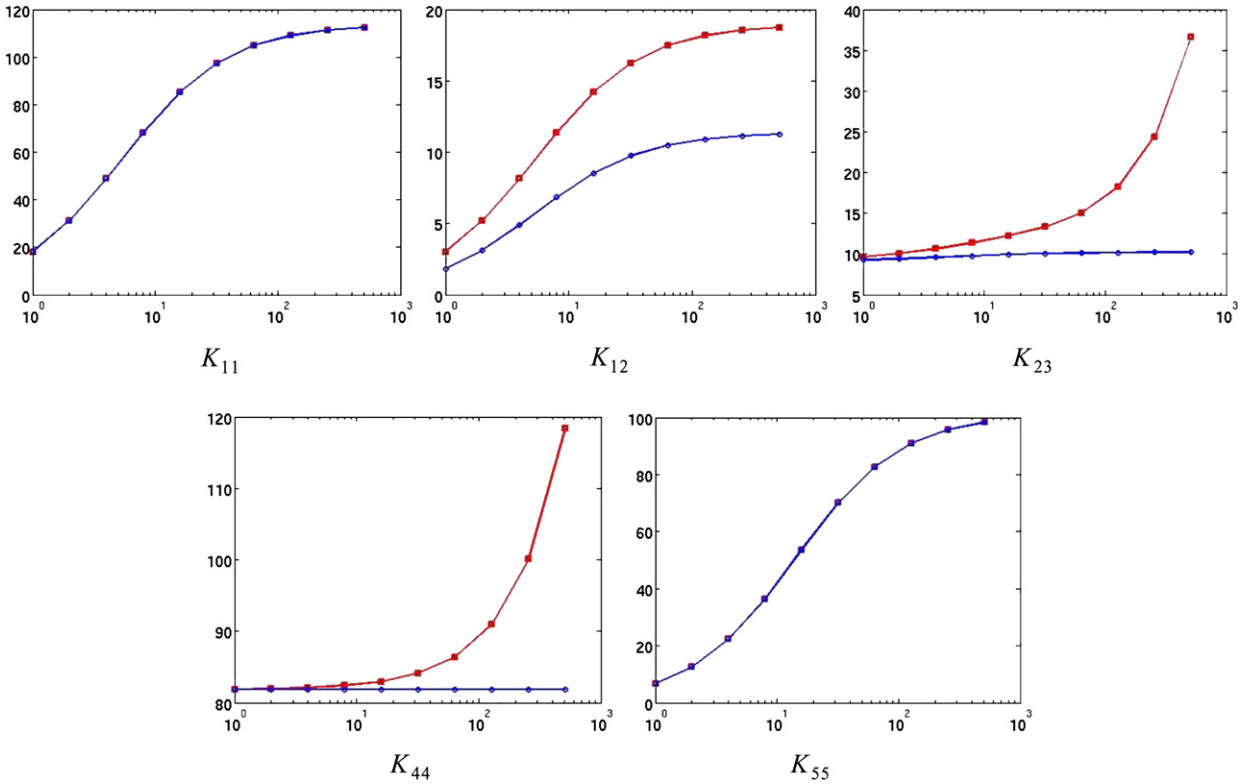

Fig. 1. Evolution of the elastic constants (GPa) of the homogenized multilayer material as a function of the interphase Young modulus (GPa) (square symbols: interphase and "enriched" interface description, diamond symbols: "simplified" interface description).

4. Conclusion and future prospects

To summarize, an "enriched" description has been proposed for the elastic interface behaviour of grain boundaries. It can be noted that this description is not limited to grain boundaries but can be used for different kinds of planar imperfect interphases. The way to derive interface properties from interphase properties, which can be heterogeneous and anisotropic, has been proposed. When dealing with an idealized multilayer material, the exact solution can be reproduced with the "enriched" description while a quite important discrepancy can be observed with the "simplified" description. The model presented in this paper can be considered as an intermediate model between the "simplified" model and the model derived by Benveniste [10].

In order to deal with "real" polycrystals (such as Voronoï polycrystals) in finite element calculations, a new interface element will have to be developed accounting for the in-plane strain of the element (which is not considered in classical interface elements). To follow the methodology proposed in [1], the interface behaviour will have to be derived from Molecular Dynamics calculations (as proposed in [3]). Finally, it is noteworthy that the derivation of an enriched description of the thermal interface behaviour is straightforward following the same arguments.

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