



HAL
open science

Modelling and simulation of multi-phase effects on X-Ray Elasticity Constants

Sylvain Fréour, David Gloaguen, Manuel François, Ronald Guillen

► **To cite this version:**

Sylvain Fréour, David Gloaguen, Manuel François, Ronald Guillen. Modelling and simulation of multi-phase effects on X-Ray Elasticity Constants. *physica status solidi (b)*, 2003, 239, pp.297-309. 10.1002/pssb.200301833 . hal-01007078

HAL Id: hal-01007078

<https://hal.science/hal-01007078>

Submitted on 15 Feb 2019

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Modelling and simulation of multi-phase effects on X-ray elasticity constants

S. Fréour^{*,1}, D. Gloaguen¹, M. François², and R. Guillén¹

¹ Laboratoire d'Applications des Matériaux à la Mécanique (L.A.M.M.), L.A.M.M.–C.R.T.T., Boulevard de L'Université, BP 406, 44602 Saint Nazaire Cedex, France

² Laboratoire des Systèmes Mécaniques et d'Ingénierie Simultanée (L.A.S.M.I.S.), Université de Technologie de Troyes, 12 Rue Marie Curie, BP 2060, 10010 Troyes, France

This paper deals with the calculation of X-ray Elasticity Constants (XEC) of phases embedded in multi-phase polycrystals. A three scales (macroscopic, pseudo-macroscopic, mesoscopic) model based on the classical self-consistent formalism is developed in order to analyse multi-phase effects on XEC values. Simulations are performed for cubic or hexagonal crystallographic structure phases embedded in several two-phases materials. In fact, it is demonstrated that XEC vary with the macroscopic stiffness of the whole polycrystal. In consequence, the constants of one particular phase depend on the elastic behaviour and the volume fraction of all the phases constituting the material. Now, XEC play a leading role in pseudo-macroscopic stresses determination by X-Ray Diffraction (XRD) methods. In this work, a quantitative analysis of the multi-phase effects on stresses determination by XRD methods was performed. Numerical results will be compared and discussed.

1 Introduction

Experimenters require proportionality constants, called X-ray Elasticity Constants (XEC), in order to determine the residual stress state of a material from X-ray strain measurements [1].

Apart from effects due to crystallites morphology or orientation (crystalline texture), XEC depend on several parameters such as the diffracting planes chosen, the nature of each phase through their elastic mechanical properties, and the volume fraction of the different phases constituting the multi-phase polycrystal [2]. Methods leading to XEC values determination are well known in the case of single-phase materials. Experimental and scale transition simulation schemes (based for example on works [3–9]) yield concordant numerical results in this particular case. For two phases materials, a more elaborate approach is proposed in the present paper. Knowing the volume fraction and the mechanical behaviour of the single crystal of each phase, one needs to calculate the XEC necessary for his experiments. In fact, it is usually assumed that XEC remain the same in two-phases materials as in single phase ones. This hypothesis yields straightforwardly to introduce the classical, available in the literature, values of single-phase XEC in the “ $\sin^2\psi$ ” relation, in order to process the experimental pseudo-macroscopic strain data obtained through measures in two-phases samples, e.g. [10–13]. This methods implicitly neglects the effects of the second phase on the mechanical elastic behaviour of the diffracting volume. It implicitly considers the phase as a connex domain in which the diffracting volume is fully embedded. The aim of this work consists in the evaluation of the two-phases effect on the XEC values and its consequences on the stresses determined by XRD analysis in cubic and hexagonal crystallographic structures.

* Corresponding author: e-mail: freour@lamm.univ-nantes.fr, Tel.: +33 02 40 17 26 25, Fax: +33 02 40 17 26 18

2 One site self-consistent calculation model

2.1 The three scales representation for multi-phase materials: scale transition formalism

XRD stress determination amounts to a sampling of the material with a set of crystallites which orientations are well defined. The elastic properties of this set are therefore anisotropic. It means that a multiscale modeling of XEC should start at the crystallite scale with an elastically anisotropic formulation. To account for intergranular heterogeneities occurring during elastic strain, self-consistent approaches are used to express the behavior of polycrystals. As part of the model, ellipsoidal inclusions, representing a crystallite, are one after another embedded in an infinite homogeneous equivalent matrix representing the two-phases polycrystalline aggregate. It should be remembered that XEC concept is based on an isotropic elastic behaviour of the matrix. It implies that the material should be assumed as perfectly disordered. In fact, in the particular case, when the principal axis of ellipsoidal anisotropic inclusions are statistically oriented, macroscopic stiffness remains isotropic, even in two-phases materials. This question has been thoroughly investigated by Qiu and Weng [14]. In the general case, however, when the principal axis are preferentially oriented along a specific direction, the elastic properties of the homogeneous equivalent medium become anisotropic. Macroscopic anisotropy can appear in the presence of crystalline texture too [15]. In the considered context, the main consequence of macroscopic anisotropy is that the classical XEC are no more suitable for the interpretation of XRD strains measurements. It will often be necessary to introduce the matrix of the stress factors, calculated from the Orientation Distribution Function (ODF). An example is given by Sprauel et al. in [16].

First, let us introduce the description of the effective macroscopic mechanical behavior (σ^I, ε^I) of the polycrystal. The statistical self-consistent framework assumes the following regular equations deduced from [6, 9, 17] :

$$\sigma^I = \mathbf{C} : \varepsilon^I, \quad \text{with} \quad \mathbf{C} = \left\langle \mathbf{c}^i(\Omega) : \left\{ \mathbf{I} + \mathbf{P} : \left[\mathbf{c}^i(\Omega) - \mathbf{C} \right]^{-1} \right\} \right\rangle_{i=1,N} \quad (1)$$

σ and ε are the stresses and strains. Superscripts I or II on strain and stress tensors denote respectively macroscopic (first order) and mesoscopic (second order) quantities.

\mathbf{C} is the effective elastic modulus of the homogeneous equivalent medium (polycrystal).

\mathbf{I} is defined by $I_{ijkl} = \frac{(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})}{2}$, where δ is the Kronecker symbol.

$\mathbf{c}^i(\Omega)$ denotes the single crystal elastic stiffness (of the phase i) referred to a sample-fixed coordinate system whose orientation, in which the orientation of the crystallite is symbolically denoted by Ω . Hill's tensor \mathbf{P} expresses the local interactions depending on the morphology assumed for the crystallites [17]. It is linked to Eshelby tensor \mathbf{S}^{esh} by $\mathbf{P} = \mathbf{C} : \mathbf{S}^{\text{esh}}$. The integration of the Green's tensor of the homogeneous equivalent medium over the surface of an inclusion provides the expression of \mathbf{P} . The method is detailed, for example, in [18].

$\mathbf{A} : \mathbf{B}$ denotes the double scalar product $A_{ijkl}B_{klmn}$.

N is the number of phases in a Representative Volume Element (RVE) of the polycrystal. It is assumed that the average of equation (1) is equivalent to a spatial average over the RVE (ergodic hypothesis). The average operation is successively done over every orientation Ω for each phase.

At mesoscopic scale, the stresses $\sigma^{II}(\Omega)$ and strains $\varepsilon^{II}(\Omega)$ of any inclusion can be expressed by a similar equation

$$\sigma^{II}(\Omega) = \mathbf{c}^i(\Omega) : \varepsilon^{II}(\Omega). \quad (2)$$

The scale transition formalism relating the macroscopic first order and mesoscopic second order mechanical states verifies the strain localization law usually described through $\varepsilon^{II}(\Omega) = \mathbf{A}(\Omega) : \varepsilon^I$, where

the localization tensor $\mathbf{A}(\mathcal{Q})$ is expressed by

$$\mathbf{A}(\mathcal{Q}) = \left[\mathbf{P} : \{ \mathbf{c}^i(\mathcal{Q}) - \mathbf{C} \} + \mathbf{I} \right]^{-1} \quad (3)$$

$\mathbf{A}(\mathcal{Q})$ depends on the macroscopic stiffness \mathbf{C} which can be calculated iteratively from the implicit equation (1).

Following Hill [8], the macroscopic strain is obtained by

$$\varepsilon^I = \langle \varepsilon^{II}(\mathcal{Q}) \rangle. \quad (4)$$

In order to study a multi-phase polycrystal, it is necessary to introduce a pseudo-macroscopic, intermediate, scale between the mesoscopic and the macroscopic ones. This new level of representation has been defined by Spruel so as to simulate the behavior of the different phases constituting the whole material [19]. Remind that the term ‘‘phase’’ is here employed in its crystallographic sense: each phase is constituted by every crystallite exhibiting the same properties (e.g. single crystal elastic constants, ...), whatever their orientation \mathcal{Q} . The pseudo-macroscopic strain of a given α phase can be defined as the average of the strains over all the crystallites composing this phase:

$$\varepsilon^\alpha = \langle \varepsilon^{II}(\mathcal{Q}) \rangle_\alpha. \quad (5)$$

The localization law can be obtained from equation (3):

$$\varepsilon^\alpha = \langle \mathbf{A}(\mathcal{Q}) : \varepsilon^I \rangle_\alpha = \langle \mathbf{A}(\mathcal{Q}) \rangle_\alpha : \varepsilon^I. \quad (6)$$

In consequence, the pseudo-macroscopic stress concentration law would be expressed through

$$\sigma^\alpha = \langle \sigma^{II}(\mathcal{Q}) \rangle_\alpha = \langle \mathbf{c}^\alpha(\mathcal{Q}) : \varepsilon^{II}(\mathcal{Q}) \rangle_\alpha = \langle \mathbf{c}^\alpha(\mathcal{Q}) : \mathbf{A}(\mathcal{Q}) \rangle_\alpha : \varepsilon^I. \quad (7)$$

Using equation (6), it comes:

$$\sigma^\alpha = \langle \mathbf{c}^\alpha(\mathcal{Q}) : \mathbf{A}(\mathcal{Q}) \rangle_\alpha : \langle \mathbf{A}(\mathcal{Q}) \rangle_\alpha^{-1} : \varepsilon^\alpha. \quad (8)$$

This relation enables us to *define* the pseudo-macroscopic stiffness corresponding to a phase with

$$\mathbf{C}^\alpha = \mathbf{C}^\alpha : \varepsilon^\alpha \quad (9)$$

Comparison between (8) and (9) leads to

$$\begin{aligned} \mathbf{C}^\alpha &= \langle \mathbf{c}^\alpha(\mathcal{Q}) : \mathbf{A}(\mathcal{Q}) \rangle_\alpha : \langle \mathbf{A}(\mathcal{Q}) \rangle_\alpha^{-1} \\ \mathbf{C}^\alpha &= \langle \mathbf{c}^\alpha(\mathcal{Q}) : \left[\mathbf{P} : \{ \mathbf{c}^\alpha(\mathcal{Q}) - \mathbf{C} \} + \mathbf{I} \right]^{-1} \rangle_\alpha : \left\langle \left[\mathbf{P} : \{ \mathbf{c}^\alpha(\mathcal{Q}) - \mathbf{C} \} + \mathbf{I} \right]^{-1} \right\rangle_\alpha^{-1}. \end{aligned} \quad (10)$$

This equation is quite different from the corresponding expression of the isolated polycrystalline single α phase macroscopic stiffness (1) because the properties of the second phase might have an influence on \mathbf{C}^α through the value of \mathbf{C} (and thus of \mathbf{P}). In fact, equation (1) is established by considering each phase as a single inclusion whereas in equation (10) each phase is composed of many crystallites with different orientations. The term $\langle \mathbf{A}(\mathcal{Q}) \rangle_\alpha^{-1} = \langle \left[\mathbf{P} : \{ \mathbf{c}^\alpha(\mathcal{Q}) - \mathbf{C} \} + \mathbf{I} \right]^{-1} \rangle_\alpha^{-1}$ might be considered as a deviation factor expressing the average interaction between α crystallites and the infinite equivalent medium. In consequence, in a multi-phase material, the nature and the proportion of the other phases forming the polycrystal affect the average elastic properties of a given α phase. As a result, the pseudo-macroscopic stiffness of a phase arbitrarily isolated might not be identified to its macroscopic stiffness, when it is integrated in a multi-phase material.

The reason why \mathbf{C}^α is not equal to its single phase value could either be a closure problem of the self-consistent model or have a physical origin. As a matter of fact, the definition of the pseudo-macroscopic stress and strain in equations (6) and (7), although intuitive and consistent with usual definitions, is arbitrary.

Basic tests can be performed to study the expressions obtained. Let us consider a single-phase material. The definition of the average strain $\varepsilon^I = \langle \varepsilon^{\text{II}} \rangle$ implies that $\langle \mathbf{A}(\mathcal{Q}) \rangle = \mathbf{I} = \langle \mathbf{A}(\mathcal{Q}) \rangle_\alpha = \langle \mathbf{A}(\mathcal{Q}) \rangle_\alpha^{-1}$. In consequence, (10) leads to the expected regular single-phase implicit relation (1):

$$\mathbf{C}^\alpha = \left\langle \mathbf{c}^\alpha(\mathcal{Q}) : \mathbf{A}(\mathcal{Q}) \right\rangle_\alpha : \left\langle \mathbf{A}(\mathcal{Q}) \right\rangle_\alpha^{-1} = \left\langle \mathbf{c}^\alpha(\mathcal{Q}) : \mathbf{A}(\mathcal{Q}) \right\rangle_\alpha = \left\langle \mathbf{c}^\alpha(\mathcal{Q}) : \left[\mathbf{P} : \{ \mathbf{c}^\alpha(\mathcal{Q}) - \mathbf{C}^\alpha \} + \mathbf{I} \right]^{-1} \right\rangle_\alpha.$$

Let us focus on the general case of a n -phases polycrystalline aggregate, containing a volume fraction f^i of any given phase i . Imposing the homogenization conditions (4) and (5) over the strain localization law (6) gives : $\langle \mathbf{A}(\mathcal{Q}) \rangle_{i=1,N} = \mathbf{I}$.

$$\text{This expression can also be developed : } f^\alpha \langle \mathbf{A}(\mathcal{Q}) \rangle_\alpha + \sum_{i \neq \alpha} f^i \langle \mathbf{A}(\mathcal{Q}) \rangle_i = \mathbf{I}.$$

In consequence, α phase average pseudo-macroscopic localization tensor deviates from the identity as follows: $\langle \mathbf{A}(\mathcal{Q}) \rangle_\alpha = \frac{1}{f^\alpha} \mathbf{I} - \frac{1}{f^\alpha} \sum_{i \neq \alpha} f^i \langle \mathbf{A}(\mathcal{Q}) \rangle_i$. Where f^i is the volume fractions of phase i and $\sum_{i=1}^N f^i = 1$.

In conclusion, self-consistent model constitutive relations imply that the average pseudo-macroscopic localization tensor of a given α phase is necessarily different from the identity. This results in a deviation between pseudo-macroscopic stiffness and the corresponding single-phase macroscopic stiffness. Also, this deviation should be considered as the expression of continuum mechanics fundamental laws rather than as an hypothetical closure problem of the model. As a matter of fact, it can be considered that the α phase is not a connex volume. One could intuitively think that its overall properties should be influenced by the medium that makes it connex. Therefore, as a response to a given average stress, the phase is not free to deform in its own ‘‘macroscopic’’ way, when it is embedded in other phases. In consequence, the deviation between single-phase macroscopic stiffness and pseudo-macroscopic stiffnesses will be strongly related to the volume fraction and elastic mechanical properties of these other phases.

The introduction of the pseudo-macroscopic stiffness \mathbf{C}^α raises the question of the scale transition relations existing between the phases and the polycrystalline multi-phase matrix. According to the strain localization (3), the macroscopic strain can be developed as follows:

$$\varepsilon^I = \mathbf{P} : \mathbf{c}^i(\mathcal{Q}) : \varepsilon^{\text{II}}(\mathcal{Q}) - \mathbf{P} : \mathbf{C} : \varepsilon^{\text{II}}(\mathcal{Q}) + \varepsilon^{\text{II}}(\mathcal{Q}). \quad (11)$$

An averaging of this expression only on α phase crystallites yields:

$$\left\langle \varepsilon^I \right\rangle_\alpha = \left\langle \mathbf{P} : \mathbf{c}^\alpha(\mathcal{Q}) : \varepsilon^{\text{II}}(\mathcal{Q}) \right\rangle_\alpha - \left\langle \mathbf{P} : \mathbf{C} : \varepsilon^{\text{II}}(\mathcal{Q}) \right\rangle_\alpha + \left\langle \varepsilon^{\text{II}}(\mathcal{Q}) \right\rangle_\alpha. \quad (12)$$

ε^I , \mathbf{P} and \mathbf{C} being constant over α phase, these tensors may be factored out of the averages:

$$\varepsilon^I = \mathbf{P} : \left\langle \mathbf{c}^\alpha(\mathcal{Q}) : \varepsilon^{\text{II}}(\mathcal{Q}) \right\rangle_\alpha - \mathbf{P} : \mathbf{C} : \left\langle \varepsilon^{\text{II}}(\mathcal{Q}) \right\rangle_\alpha + \left\langle \varepsilon^{\text{II}}(\mathcal{Q}) \right\rangle_\alpha. \quad (13)$$

According to the mesoscopic to pseudomacroscopic averaging equations (5) and (7), one should obtain:

$$\varepsilon^I = \mathbf{P} : \sigma^\alpha - \mathbf{P} : \mathbf{C} : \varepsilon^\alpha + \varepsilon^\alpha = \mathbf{P} : \mathbf{C}^\alpha : \varepsilon^\alpha - \mathbf{P} : \mathbf{C} : \varepsilon^\alpha + \varepsilon^\alpha = \left[\mathbf{P} : \{ \mathbf{C}^\alpha - \mathbf{C} \} + \mathbf{I} \right] : \varepsilon^\alpha. \quad (14)$$

Finally, the pseudomacroscopic stresses and strains can be expressed through the macroscopic strain state, as a function of the pseudomacroscopic and macroscopic stiffness, respectively given by (14)

and (9):

$$\varepsilon^\alpha = \left[\mathbf{P} : (\mathbf{C}^\alpha - \mathbf{C}) + \mathbf{I} \right]^{-1} : \varepsilon^I, \quad (15)$$

$$\sigma^\alpha = \mathbf{C}^\alpha : \left[\mathbf{P} : (\mathbf{C}^\alpha - \mathbf{C}) + \mathbf{I} \right]^{-1} : \varepsilon^I. \quad (16)$$

These equations mean that the average stress or strain state of the polycrystalline α -phase can be obtained through a classical multi-phase self-consistent scheme by considering it as a single inclusion of stiffness \mathbf{C}^α embedded in a homogeneous matrix having the stiffness of the macroscopic material. However, it should be remembered that the stiffness tensor \mathbf{C}^α is not that of the isolated single α -phase but is given by equation (10). Up to now, the developed equations are very general. They are therefore valid for a macroscopically anisotropic (textured) material.

Finally, in order to take into account multi-phase effects in the simulation, it is necessary to consider three levels in the schematization of the material: the classical grain and polycrystal levels (mesoscopic and macroscopic scales) and an intermediate pseudo-macroscopic scale defining the behaviour of each phase. This representation and the associated scale transition formalism will now be applied to XEC determination.

2.2 Application to XEC simulation

According to [16, 20], the lattice strain $\varepsilon_{\varphi,\psi}^\alpha$ measured in α phase by XRD corresponds to the integration of the mesoscopic strains (3) over all orientations Ω of the Diffracting Volume (DV), and their projection on the measurement direction φ, ψ :

$$\varepsilon_{\varphi,\psi}^\alpha = \bar{n}^I \cdot \left\langle \varepsilon^{\text{II}}(\Omega) \right\rangle_{\alpha, \text{DV}} \cdot \bar{n}, \quad \text{with} \quad \bar{n} = \begin{pmatrix} \sin \psi \cos \varphi \\ \sin \psi \sin \varphi \\ \cos \psi \end{pmatrix}. \quad (17)$$

Neglecting effects due to crystallographic or morphologic texture, the usual linear relation between the measured strain and the triaxial pseudo-macroscopic stress undergone by the α -phase could be developed as follows :

$$\begin{aligned} \varepsilon_{\varphi,\psi}^\alpha &= \frac{1}{2} S_2^\alpha \left(\sigma_{11}^\alpha \cos^2 \varphi + \sigma_{12}^\alpha \sin 2\varphi + \sigma_{22}^\alpha \sin^2 \varphi - \sigma_{33}^\alpha \right) \sin^2 \psi \\ &\quad + \frac{1}{2} S_2^\alpha \left(\sigma_{13}^\alpha \cos \varphi + \sigma_{23}^\alpha \sin \varphi \right) \sin 2\psi \\ &\quad + \frac{1}{2} S_2^\alpha \sigma_{33}^\alpha + S_1^\alpha \left(\sigma_{11}^\alpha + \sigma_{22}^\alpha + \sigma_{33}^\alpha \right). \end{aligned} \quad (18)$$

Substituting the numerical values obtained through (16, 17) in (18) provides a relation leading to the determination of the XEC $1/2 S_2^\alpha$ and S_1^α characteristic of the α -phase embedded in the multi-phase polycrystal studied.

According to the theory described by Bollenrath, Hauk and Müller [21], the XEC of a given cubic symmetry phase can be expressed for any $\{hkl\}$ diffracting plane through: $\frac{1}{2} S_2(hkl) = \frac{1}{2} S_2(h00) - 3\Gamma(hkl)S$. This expression depends on two main factors: the slope S , and the cubic orientation parameter symbolically denoted by Γ . These terms are respectively given by:

$$\Gamma(hkl) = \frac{h^2 k^2 + h^2 l^2 + k^2 l^2}{(h^2 + k^2 + l^2)^2}, \quad \text{and} \quad S = \frac{1}{2} S_2(hhh) [A_{\text{XRD}} - 1].$$

Table 1 Cubic symmetry single-crystal elasticity constants and anisotropy parameter A_c .

	austenitic phase [23]	ferritic phase [23]	aluminium [1]	β -SiC [23]	diamond-C [23]	copper [1]
c_{11} [GPa]	197.5	237.4	108.2	352.3	1020.0	168.4
c_{12} [GPa]	124.5	134.7	61.3	140.4	250.0	121.4
c_{44} [GPa]	122.0	116.4	28.5	232.9	390.0	75.4
$A_c = \frac{2c_{44}}{c_{11} - c_{12}}$	3.34	2.27	1.23	2.20	1.01	3.21

A_{XR} denotes the X-Ray anisotropy coefficient of the diffracting phase, corresponding to the following ratio: $A_{XR} = \frac{\frac{1}{2}S_2(h00)}{\frac{1}{2}S_2(hhh)}$.

In the same way, XEC of hexagonal symmetry phases verify the following relation due to Evenschor and Hauk [19]: $\frac{1}{2}S_2(hk.l) = x_1 + x_2H(hk.l) + x_3H^2(hk.l)$.

Introducing the lattice parameters a and c of the considered structure, the hexagonal orientation parameter symbolically denoted by H is given by: $H(hk.l) = \frac{l^2}{\frac{4}{3}\left(\frac{c}{a}\right)^2(h^2 + k^2 + hk) + l^2}$.

In consequence, for phases exhibiting hexagonal crystallographic structure, $1/2 S_2$ values varies between $1/2 S_2(10.0) = x_1$ and $1/2 S_2(00.1) = x_1 + x_2 + x_3$.

This model has been used to simulate the cases of several two-phases materials: duplex steels, aluminium- β silicon carbide Metal Matrix Composites (MMC), aluminium-diamond carbon composites, copper- Fe_α alloys, aluminium-beryllium alloys, aluminium-zinc alloys and cadmium-zinc alloys. The different systems have been especially chosen in order to separate the effects of the following parameters on XEC values: single-crystal anisotropy, crystallographic structure and the ratio of the elastic moduli of the two considered phases.

The micromechanical constants used for each cubic or hexagonal single-crystal inclusion are respectively given in Tables 1 and 2. The two-phases elastic behaviour has been simulated through a calculus involving 4000 spherical crystallites randomly oriented. The diffracting volume elastic behaviour has then been determined for each phase and different compositions of the $\alpha + \beta$ material: 0% β , 25% β , 50% β , 75% β and 100% β , (this last composition corresponds to the limiting case of vanishing α phase). Table 3 summarizes the cases of two usually encountered materials: duplex steels and aluminium- β silicon carbide MMC. The localization of a macroscopic stress in the crystallites of the diffracting volume provides values for the XEC. Results obtained are given in Tables 4 and 5 which summarizes the main elastic heterogeneities and sources of anisotropy of the considered polycrystals. Nevertheless, XEC do not depend on σ . In consequences, the macroscopic loading is arbitrary.

Table 2 Hexagonal symmetry single-crystal elasticity constants [25].

	c_{11} [GPa]	c_{12} [GPa]	c_{13} [GPa]	c_{33} [GPa]	c_{44} [GPa]	c_{66} [GPa]	A_{h1}	A_{h2}	c_{11}/c_{33}
zinc	165.0	31.0	50.0	62.0	39.6	67.0	1.64	0.39	2.66
cadmium	114.5	39.5	39.9	50.8	19.8	37.5	1.89	0.66	2.24
beryllium	292.3	26.7	14.0	336.4	162.5	132.8	0.82	0.94	0.87

NB: The departure of the parameters A_{h1} , A_{h2} and c_{11}/c_{33} from unity can be used as a measure of the elastic anisotropy of hexagonal crystals.

Table 3 Multi phase effects on pseudomacroscopic stiffness.

Stiffness tensor components and bulk moduli calculated in Al–SiC MMC at pseudomacroscopic scale					
$f(\text{Al})$	0.00	0.25	0.50	0.75	1.00
$C_{11}(\text{Al})$ [GPa]	112.2	112.2	112.1	112.1	112.1
$C_{12}(\text{Al})$ [GPa]	59.3	59.3	59.3	59.3	59.4
$K(\text{Al})$ [GPa]	76.9	76.9	76.9	76.9	77.0
$C_{11}(\text{SiC})$ [GPa]	437.7	434.2	430.8	428.1	426.7
$C_{12}(\text{SiC})$ [GPa]	97.6	99.4	101.1	102.5	103.2
$K(\text{SiC})$ [GPa]	211.0	211.0	211.0	211.0	211.0

Stiffness tensor components and bulk moduli calculated in duplex steels at pseudomacroscopic scale					
$f(\text{Fe}_\alpha)$	0.00	0.25	0.50	0.75	1.00
$C_{11}(\text{Fe}_\alpha)$ [GPa]	281.0	281.1	281.2	281.2	281.2
$C_{12}(\text{Fe}_\alpha)$ [GPa]	112.9	112.8	112.8	112.8	112.7
$K(\text{Fe}_\alpha)$ [GPa]	168.9	168.9	168.9	168.9	168.9
$C_{11}(\text{Fe}_\gamma)$ [GPa]	250.6	250.8	251.1	251.3	251.5
$C_{12}(\text{Fe}_\gamma)$ [GPa]	97.9	97.8	97.7	97.6	97.5
$K(\text{Fe}_\gamma)$ [GPa]	148.8	148.8	148.8	148.8	148.8

Table 4 XEC [10^{-6}MPa^{-1}] determined in cubic symmetry phases of several two-phases polycrystals.

XEC calculated in the case of a MMC aluminium– β silicon carbide						
diffracting phase volume fraction		100%	75%	50%	25%	~0%
aluminium	$1/2 S_2(h00)$	19.99	19.75	19.52	19.31	19.19
	S	1.71	1.35	0.98	0.69	0.49
β -SiC	$1/2 S_2(h00)$	3.63	3.82	4.04	4.23	4.36
	S	1.15	1.40	1.68	1.93	2.10

XEC calculated in the case of duplex steel						
diffracting phase volume fraction		100%	75%	50%	25%	~0%
austenitic phase	$1/2 S_2(h00)$	8.77	8.68	8.65	8.59	8.56
	S	3.68	3.59	3.54	3.48	3.43
ferritic phase	$1/2 S_2(h00)$	7.31	7.33	7.35	7.37	7.41
	S	2.29	2.32	2.34	2.39	2.43

XEC calculated in the case of an iron–copper two-phases polycrystal						
diffracting phase volume fraction		100%	75%	50%	25%	~0%
ferritic phase	$1/2 S_2(h00)$	7.31	7.39	7.56	7.71	7.82
	S	2.29	2.43	2.61	2.80	2.96
copper	$1/2 S_2(h00)$	13.55	13.32	12.94	12.55	12.34
	S	5.36	5.00	4.57	4.15	3.84

XEC calculated in the case of an aluminium–diamond carbon two-phases polycrystal						
diffracting phase volume fraction		100%	75%	50%	25%	~0%
aluminium	$1/2 S_2(h00)$	19.99	19.69	19.34	19.11	19.06
	S	1.71	1.23	0.70	0.37	0.23
diamond carbon	$1/2 S_2(h00)$	1.29	1.29	1.30	1.30	1.30
	S	0.01	0.01	0.01	0.01	0.01

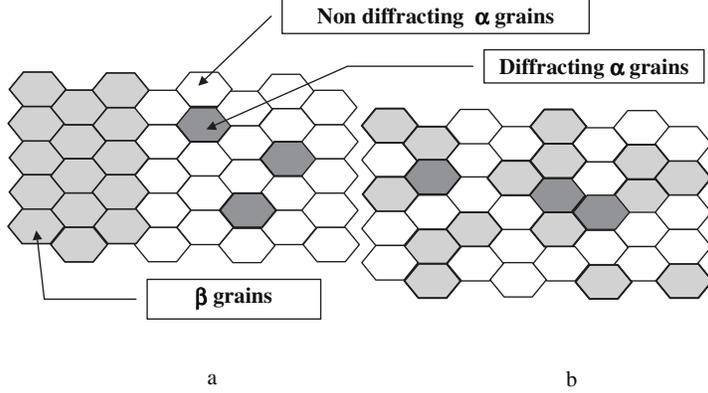


Fig. 1 a) Diffracting volume constituted by α grains only connected to other α grains. (Case of equality of the XEC in the single-phase and two-phases material). b) Diffracting volume constituted of α grains interacting with α and β first neighbours grains.

3 Interphase interactions in two-phases polycrystals

3.1 Discussion about multi-phase effects on pseudomacroscopic stiffness values (Table 3)

The one site self consistent formalism (10) shows that the pseudo-macroscopic stiffness tensor of a given phase integrated in a multi-phase material should be different from the corresponding single-phase material macroscopic stiffness. Pseudo-macroscopic stiffness obviously varies as a function of the nature and volume fraction of the other phase constituting the two-phases polycrystal. Nevertheless, it is shown in table 3 that, in most cases, multi phase effect on pseudo-macroscopic stiffness is usually negligible. Although pseudo-macro-stiffness varies with the nature and the volume fraction of the other phase, the bulk modulus K of each phase remains perfectly constant at pseudomacroscopic scale. It is well known that K

Table 5 XEC [10^{-6} MPa $^{-1}$] determined in hexagonal symmetry phases of several two-phases polycrystals

XEC calculated in the case of an aluminium–beryllium two-phases polycrystal						
diffracting phase volume fraction		100%	75%	50%	25%	~0%
beryllium	$x_1 = 1/2 S_2(10.0)$	3.52	3.55	3.58	3.60	3.62
	x_2	-0.68	-0.79	-0.90	-0.98	-1.03
	x_3	0.39	0.44	0.47	0.48	0.47
	$1/2 S_2(00.1)$	3.23	3.20	3.15	3.10	3.06
XEC calculated in the case of a cadmium–zinc two-phases polycrystal						
diffracting phase volume fraction		100%	75%	50%	25%	~0%
cadmium	$x_1 = 1/2 S_2(10.0)$	17.72	17.80	17.90	17.97	18.05
	x_2	5.74	5.80	5.76	5.62	5.43
	x_3	6.37	5.16	4.14	3.28	2.61
	$1/2 S_2(00.1)$	29.83	28.76	27.80	26.87	26.09
zinc	$x_1 = 1/2 S_2(10.0)$	10.21	10.21	10.23	10.24	10.27
	x_2	- 0.84	- 1.26	- 1.80	- 2.43	- 3.17
	x_3	8.61	9.83	11.28	12.90	14.71
	$1/2 S_2(00.1)$	17.98	18.78	19.71	20.71	21.81
XEC calculated in the case of an aluminium–zinc two-phases polycrystal						
diffracting phase volume fraction		100%	75%	50%	25%	~0%
zinc	$x_1 = 1/2 S_2(10.0)$	10.21	10.21	10.21	10.22	10.24
	x_2	- 0.84	- 1.24	- 1.75	- 2.38	- 3.19
	x_3	8.61	9.73	11.05	12.60	14.51
	$1/2 S_2(00.1)$	17.98	18.70	19.51	20.44	21.56

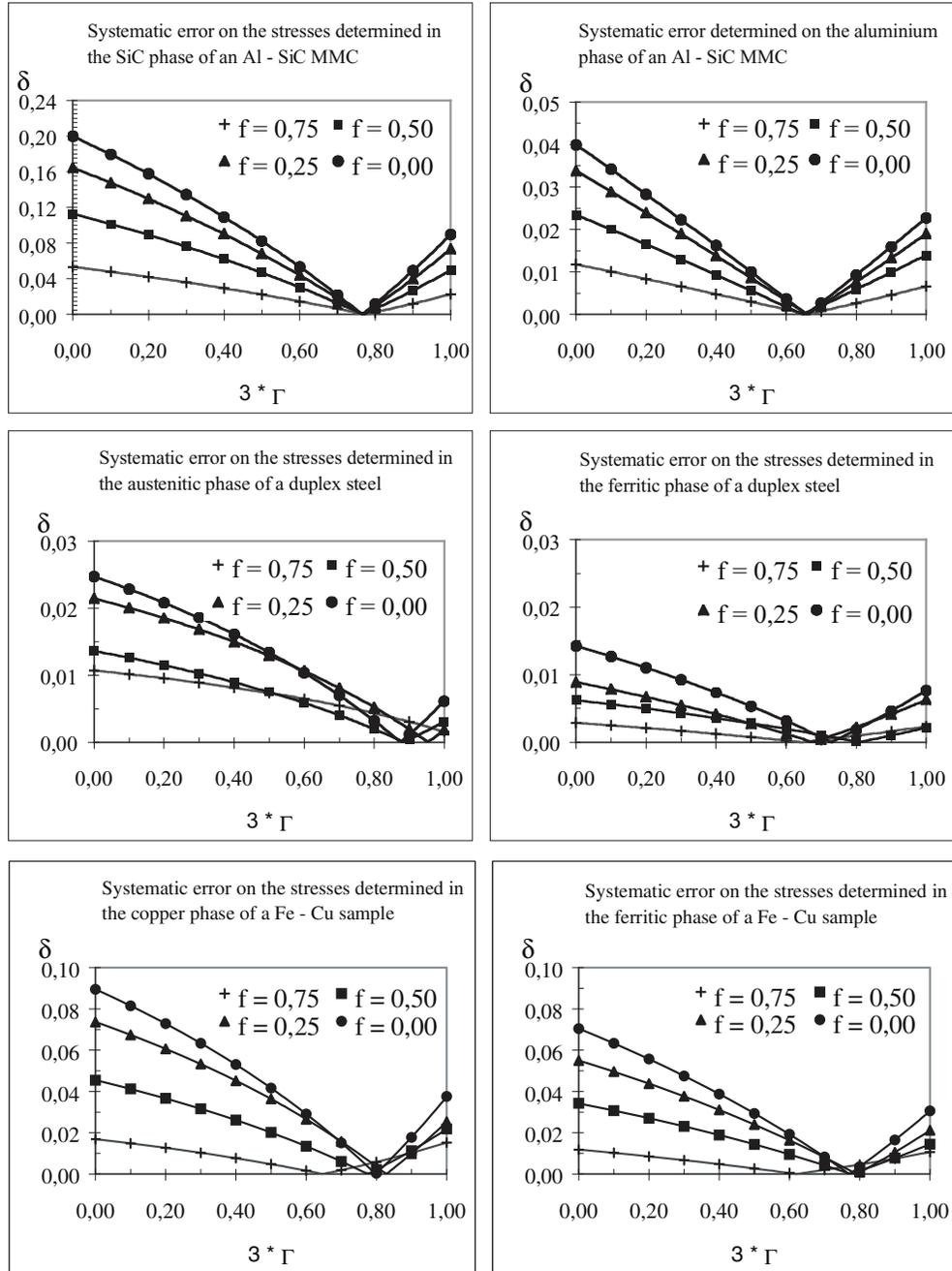


Fig. 2 Calculated systematic relative error δ , due to multiphase effects, on the stresses determined in several cubic structure phases of two-phases polycrystals. f denotes the volume fraction of the analysed phase. $\delta(f=0)$ corresponds to the limit case of Eshelby's inclusion. These values constitute the upper bound of the systematic error.

values are, since it is an invariant of the stiffness tensor, identical in single crystal (mesoscopic scale) and in cubic structure single phase polycrystals (macroscopic scale). In consequence a variation of the bulk modulus would not be physically acceptable. Results obtained satisfy this criterion. This confirms the numerical validity of the model developed which implies the deviation of pseudo macro stiffness values

in order to ensure the consistence between the average moduli determined at macroscopic and pseudo-macroscopic scales, and the elastic behaviour of the inclusions.

3.2 Analyse of multi-phase effects on XEC

Tables 4, 5 show that the XEC of a given α -phase generally vary with the volume fraction of the phase in a given system, and with the nature of the second (β) phase. The model takes into account multi-phase effects on XEC numerical values. In physical terms, this discrepancy between XEC of a given phase, calculated in a single-phase material and in a two phases sample can be explained by the elastic interactions existing between the polycrystalline matrix and any crystallite. Through these interactions, the mechanical behaviour of α -phase diffracting volume depends directly on the polycrystalline macroscopic stiffness denoted by C . Thus, according to (1), the second phase is closely involved in the iterative calculation of C tensor. In consequence, the presence of the β -phase affects α -phase diffracting volume mechanical behaviour through its volume fraction and pseudo-macroscopic stiffness C^β tensor. This phenomenon can be schematised on Fig. 1a and 1b: α -phase XEC could be equal in the single-phase sample and in the two-phases polycrystal, if the crystallites of α diffracting volume were only connected to α grains. This corresponds to the Fig. labelled 1a. As part of this particular assumption, an α diffracting inclusion interacts only with a homogeneous medium having a macroscopic stiffness close to C^α . How

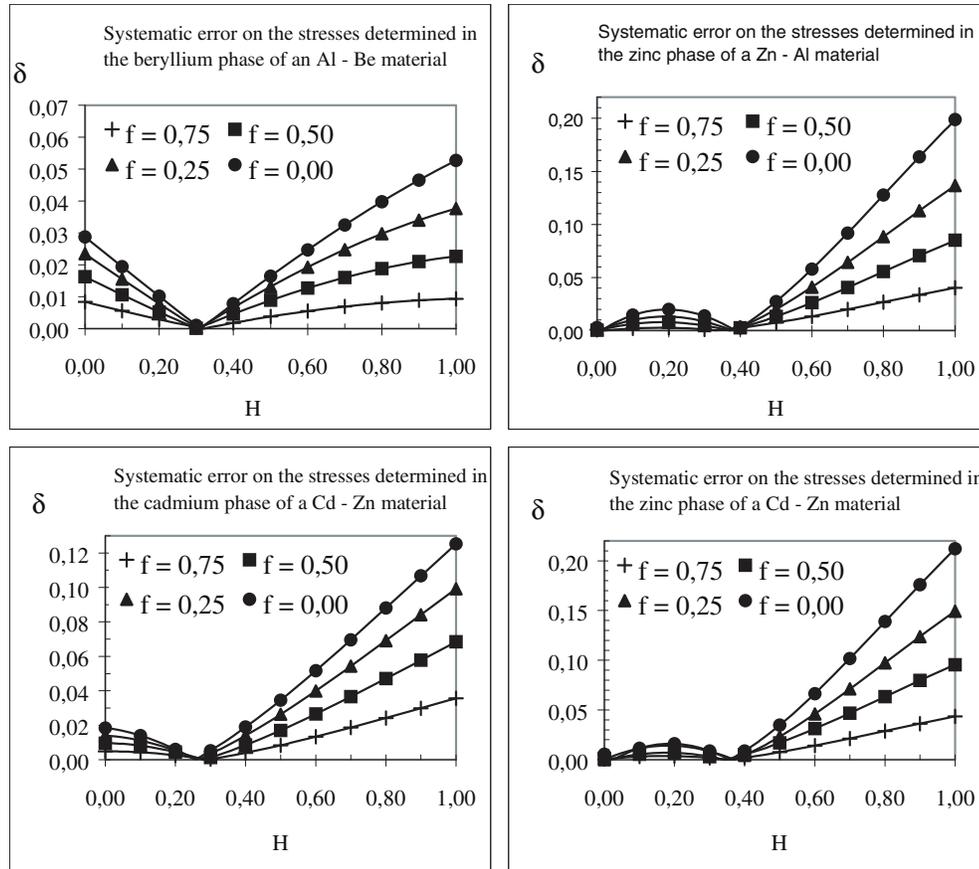


Fig. 3 Calculated relative systematic error δ , due to multiphase effects, on the stresses determined in several hexagonal structure phases of two-phases polycrystals. f denotes the volume fraction of the analysed phase.

ever, in reality, the grains of α diffracting volume often have α and β grains as first neighbours simultaneously, as shown on Fig. 1 b. The presence of these first neighbours β grains generates interactions which affect α diffracting volume elastic behaviour. In fact, our model only describes the case of Fig. 1 b in an average meaning: the interactions of β grains on the behaviour of α phase are only taken into account through the average stiffness of the matrix, i.e. the homogeneous equivalent medium.

In the case of the MMC aluminium– β SiC, calculated XEC strongly depend on each phase volume fraction. Similar effects have been observed for several two-phases polycrystals: in pure cubic structure systems in the case of ferritic steel–copper sample, in pure duplex hexagonal structure such as cadmium–zinc polycrystal, and in dual structure systems, in the case of aluminium–zinc polycrystal, for example. This property, characteristic to such two-phases polycrystals, results from the mechanical behaviour heterogeneities existing between the phases.

On the opposite, when the macroscopic behaviour of the two phases is similar, such as in the case of duplex steels, the XEC do not vary significantly with the volume fraction of each phase.

In conclusion, in a $(\alpha + \beta)$ two-phases polycrystal, the XEC of a given α -phase deviates more and more from the values obtained in the single-phase case, when α -phase volume fraction tends towards 0, and when α and β have very different elastic behaviour.

In the case of aluminium–diamond like carbon systems, aluminium XEC verify this rule, while diamond XEC seem not to follow it. In fact, diamond XEC remains almost constant, in spite of the large mechanical discrepancies existing between the two phases. This result could be expected in particular cases: a phase with elastically isotropic single crystal keeps its XEC constant, whatever the two-phases state of the polycrystal in which it is embedded. In fact, this property is only valid for a macroscopically isotropic material. If the second phase exhibit a crystallographic or morphologic texture, the overall stiffness tensor will be anisotropic. This would influence the localisation tensor and thus the elastic behaviour of the diffracting volume. Diamond like carbon has a single-crystal anisotropy constant A_c close to 1. In consequence, its XEC are not modified by the polycrystal two-phases state. Similar results have been obtained on tungsten ($A_c = 0.98$) and to some extent in the case of molybdenum ($A_c = 0.91$) and TiC ($A_c = 0.90$), according to the single-crystal elastic constants given in [23–25]. On the opposite, results obtained on Zinc and Copper emphasize that multi-phases effects on XEC arise in the case of strongly anisotropic diffracting phases.

4 Consequences on the stresses determined by XRD analysis on multi-phase samples

As mentioned before, the usual assumption consists in introducing single-phase XEC values in the “ $\sin^2\psi$ ” equation, in order to process numerically the strains measured in two-phases polycrystals. The results given by our simulations demonstrate that this approach constitutes an approximation of the polycrystalline sample mechanical effective behaviour. In consequence, this assumption generates a systematic error δ on the determined stresses. For a given set of $\{hkl\}$ diffracting planes, in the case of a material including a volume fraction f of the analysed phase, one should express this systematic deviation as follow :

$$\delta = \frac{\frac{1}{2}S_2(f) - \frac{1}{2}S_2(f=1)}{\frac{1}{2}S_2(f=1)}. \quad (19)$$

This relation applied to several two-phases systems yields the curves given on Figs. 2 and 3. As part of a residual stress analysis through XRD, the relative error on stresses values due to experimental and data processes generally remains between 5% and 15% for the considered phases. The maximal influence of non diffracting phase on the X-ray behaviour of diffracting phase is given in Table 6, where the main properties of the two-phases material simulated are summarized. Figs. 2 and 3 show that the systematic relative error δ resulting from the usual assumption is often lower than 5%. δ curves confirm the existence of particular Γ_0 orientation values for which XEC are equal in the single phase and in the two-phases material.

Table 6 Maximum multi-phase influence on XEC.

material	diffracting phase	crystallographic structure	diffracting phase anisotropy	non diffracting phase anisotropy	ratio of moduli of the two phases	maximum influence of not diffracting phase on the X-ray behaviour of diffracting phase (δ_{\max})
Fe($\alpha + \beta$)	Fe(α)	cubic	medium	strong	weak	1.4%
	Fe(γ)	cubic	strong	medium		2.4%
Fe(α)/Cu	Fe(α)	cubic	medium	strong	medium	7.0%
	Cu	cubic	strong	medium		8.9%
Al/SiC	Al	cubic	weak	medium	strong	4.0%
	SiC	cubic	medium	weak		20.1%
Al/C	Al	cubic	weak	none	strong	4.7%
	C	cubic	none	weak		0.1%
Al/Be	Al	cubic	weak	weak	strong	3.3%
	Be	hexagonal	weak	weak		5.3%
Al/Zn	Al	cubic	weak	strong	medium	1.1%
	Zn	hexagonal	strong	weak		19.9%
Cd/Zn	Cd	hexagonal	medium	strong	medium	12.5%
	Zn	hexagonal	strong	medium		21.3%

It should be noted that our purpose is not to obtain the macroscopic strain in a two phases material. This objective would be limited to a purely elastic loading and could not give any valuable information in the case of residual stresses due to stress-free strains such as thermal or plastic loading or phase transformation (see for example [19]). Our purpose is to provide a rigorous scheme to express the average stress of one phase of a multiphase material from the elastic strains measured by XRD in the same phase, whatever the physical origin of the stress.

To express this mathematically, the measured strain in α -phase can be expressed by

$$\varepsilon_{\varphi,\psi}^{\alpha} = \left(\mathbf{B}_1 : \sigma^{\alpha} \right)_{\phi_{\psi}},$$

$$\varepsilon_{\varphi,\psi}^{\alpha} = \left(\mathbf{B}_1 : \left[\mathbf{B}_2 : \sigma^I + \mathbf{B}_3 : \left(\varepsilon^{LI} - \varepsilon^{LaDv} \right) \right] \right)_{\phi_{\psi}}.$$

Our model provides a mean to calculate operator \mathbf{B}_1 in order to measure σ^{α} but, in no way, the expression of operators \mathbf{B}_2 and \mathbf{B}_3 nor any access to the macroscopic stress σ^I and the stress-free strains ε^{LI} and ε^{LaD} . ε^{LI} and ε^{LaDv} are respectively the macroscopic stress-free strain and the stress-free strain of α diffracting volume. In our model, the basic assumption is that one crystallite of the diffracting phase interacts with both phases in proportion to their volume fraction, however, in reality, this might not always be true. For instance, SiC particles in Al/SiC composite are composed of several crystallites; one crystallite is thus surrounded by more SiC crystallites than Al crystallites. To go a little further, the elementary domain in XRD is not the grain but the coherently diffracting domain which size is much smaller than the grain size. Whether such a domain interacts with both phases can be discussed.

5 Conclusion

The choice of the XEC values is crucial, especially so as to determine residual stress through XRD analysis. A one-site elastic self-consistent calculation scheme based on Kröner-Eshelby's formalism has been developed in order to simulate the diffracting volume elastic behaviour of cubic or hexagonal phases embedded in two-phases polycrystals. It was shown that XEC values of a given phase generally

depend on the volume fraction and pseudo-macroscopic stiffness of the other phases constituting the whole material. It has been demonstrated that this dependence could be regarded as an error source affecting the calculation of stresses from measured strains data. It is also necessary to take into account effects due to two-phases interactions in order to minimize the deviation between the residual stresses determined through XRD experiments and true stresses in the sample. To go deeper into this study, an analytical model will be soon proposed in order to express XEC for cubic phases embedded in multi-phase polycrystals. The property of elastically isotropic phases at mesoscopic scale, whose XEC remains identical to the corresponding single-phases values, in any multi-phase material, will be demonstrated owing to this analytical solution.

The deviation between pseudomacroscopic and single-phase stiffnesses was also studied. Numerical computations justifies, in most cases, the identification of pseudomacroscopic elastic moduli to the single phases corresponding values. In a further study, it will be taken advantage of this property in order to propose a method suited for the characterization of the macroscopic elastic moduli of a phase embedded in a multiphase polycrystal.

References

- [1] I. Noyan and J. Cohen, *Residual Stress Measurement by Diffraction and Interpretation* (Springer Verlag, New York, 1987).
- [2] K. Tanaka, Y. Akiniwa, and T. Ito, *Proc. of the ECRS6*, Vol. 2, 1012–1019 (2000).
- [3] W. Voigt, *Lehrbuch der Kristallphysik* (Teubner, Leipzig/Berlin, 1928).
- [4] W. Voigt, *Ann. Phys. Chem. (Leipzig)* **38**, 573–587 (1889).
- [5] A. Reuss, *Z. Angew. Math. Mech.* **9**, 49–58 (1929).
- [6] E. Kröner, *Z. Physik* **151**, 504–518 (1958).
- [7] E. Kröner, *J. Mech. Phys. Solids* **15**, 319–329 (1967).
- [8] R. Hill, *J. Mech. Phys. Solids* **15**, 79–95 (1967).
- [9] J. D. Eshelby, *Proc. R. Soc. Lond.* **241 A**, 376–379 (1957).
- [10] P. Hadmar, P. Mabelly, L. Barralier, and J. M. Sprauel, *Proc. ECRS 4*, Cluny, 1043–1051 (1996).
- [11] K. Van Acker and P. Van Houtte, *Proc. ECRS 4*, Cluny, 911–920 (1996).
- [12] M. Ceretti and C. Braham, *Colloque de métallurgie*, Saclay, 221–232 (1994).
- [13] V. Hauk, P. J. T. Stuitje, in: *Residual Stresses*, edited by E. Macherauch and V. Hauk (DGM, Oberursel, 1986), pp. 337–346.
- [14] Y. P. Qiu and G. J. Weng, *Int. J. Solids Struct.* **27**, 1537–1550 (1991).
- [15] C. Tomé, *Texture and Anisotropy* (Cambridge University Press, Cambridge, 1998), pp. 283–325.
- [16] J. M. Sprauel, M. François and M. Barral, *Proc. ICRS 2*, Nancy, 172–177 (1988).
- [17] R. Hill, *J. Mech. Phys. Solids* **13**, 89–101 (1965).
- [18] R. Morris, *Int. J. Eng. Sci.* **8**, 49–61 (1970).
- [19] J. M. Sprauel, in “Analyse des contraintes résiduelles par diffraction des rayons X et des neutrons”, (Commissariat à l’Energie Atomique, 1996), chapter VIII, pp. 185–202.
- [20] J. M. Sprauel and L. Castex, *Proc. EPDIC 1* (1991).
- [21] F. Bollenrath, V. Hauk, and E. H. Müller, *Z. Metallkde.* **58**, 76–82 (1967).
- [22] P. D. Evenschor and V. Hauk, *Z. Metallkde.* **63**, (1972).
- [23] D. H. Chung and W. R. Buessem, *J. Appl. Phys.* **39**, 217–245 (1967).
- [24] G. Simmons and H. Wang, *Single Crystal Elastic Constants and Calculated Aggregate Properties* (The M.I.T. Press, Cambridge, Mass., 1971).
- [25] W. F. Hosford, *The Mechanics of Crystals and Textured Polycrystals* (Oxford Science Publications, Oxford, 1993), p. 16.