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THIRD-ORDER ELASTIC COEFFICIENTS AND LOGARITHMIC STRAIN IN FINITE ELEMENT MODELLING OF ANISOTROPIC ELASTICITY

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1. Introduction

Contrary to higher order elastic constants for momentum stresses the second (classical) and third-order elastic coefficients (TOEC) for symmetric elasticity are measured and tabulated successfully with good accuracy for tens of years. In the classical experimental measurements of TOEC, the correct recalculation of instantaneous stiffness changes onto TOEC has an important role. A similar problem arises in the constitutive and finite element (FE) modelling. Namely, because of a very strong dependency of TOEC on the strain measure choice, the constitutive and FE modelling of elastic materials is considered here in terms of different finite strain measures. To this aim, the known analytical formulae for calculation of two first derivatives of the isotropic tensor function of tensor variable are verified by means of the finite difference method. In result, the revised formulae are used for calculation of the tangent stiffness matrix. This paper closes with some remarks on the use of TOEC in finite element modelling.

2. Third-order elastic coefficients

TOEC are often determined from ab-initio calculation as well as by measurement the effect of stress on the ultrasonic wave speeds in crystals. Usually, the coefficients are determined in relation to the Green strain [1, 4, 3]. Assume the following strain energy function for elastic material

$$\psi(\hat{\boldsymbol{\varepsilon}}) = \frac{1}{\hat{\rho}}\left[\frac{1}{2!}\hat{c}_{\ddot{y}\,kl}\,\hat{\varepsilon}^{\,\ddot{y}}\,\hat{\varepsilon}^{kl} + \frac{1}{3!}\widehat{C}_{\ddot{y}\,kl\,mn}\,\hat{\varepsilon}^{\ddot{y}}\,\hat{\varepsilon}^{kl}\,\hat{\varepsilon}^{mn}\right], \tag{1}$$

where $\widehat{\mathbf{c}}$ and $\widehat{\mathbf{C}}$ are tensors of the second- and third-order elastic coefficients determined in relation to a given strain measure; $\hat{\rho}$ is the mass density in the reference configuration. Each of strain measures from the Seth-Hill family can be recalculated to another one from the same family, according to the transformation rule

$$\hat{\boldsymbol{\varepsilon}}'(\hat{\boldsymbol{\varepsilon}}) = \begin{cases} \dfrac{1}{m'}\left[(m\hat{\boldsymbol{\varepsilon}}+\mathbf{1})^{m'/m}-\mathbf{1}\right] & \text{for} \quad m\neq 0 \wedge m'\neq 0, \\ \dfrac{1}{m'}\left[\exp\left(m'\boldsymbol{\varepsilon}\right)-\mathbf{1}\right] & \text{for} \quad m=0 \wedge m'\neq 0, \\ \dfrac{1}{m}\ln\left(m\hat{\boldsymbol{\varepsilon}}+\mathbf{1}\right) & \text{for} \quad m\neq 0 \wedge m'=0, \end{cases} \tag{2}$$

where m is the real number taking a role of an additional elastic constant. For fixed second-order elastic coefficients the instantaneous stiffness of anisotropic Hookeans in the relaxed configuration is invariant with respect to the choice of the finite strain measure. Contrary to that, TOEC corresponding to the given instantaneous stiffness curve depend very strongly on the strain measure choice. In other words, two experimenters measuring the same instantaneous stiffness change under loading can determine two dramatically different sets of TOEC dependently on the strain measure used. Simultaneously, both of

them can speak on quite the same change of instantaneous stiffness under loading. In order to hold the same instantaneous stiffness evolution in vicinity of the relaxed state, TOEC must be recalculated to the equivalent values corresponding to the strain measure used, for the Seth-Hill strain measures the formula for recalculation takes form

$$\widehat{C}'_{ij\,kl\,mn} = \widehat{C}_{ij\,kl\,mn} + (m-m')\big[\mathcal{J}_{ij\,kl}{}^{æ}\ \hat{c}_{æ\,mn} + \mathcal{J}_{kl\,mn}{}^{æ}\ \hat{c}_{æ\,ij} + \mathcal{J}_{mn\,ij}{}^{æ}\ \hat{c}_{æ\,kl}\big], \tag{3}$$

where $\boldsymbol{\mathcal{J}}$ is the sixth-order proper-symmetric unit tensor. As an example, consider the instantaneous stiffness changes for silicon crystal originally recalculated onto TOEC for Green strain by Johal and Dunstan [3], see Table 1 for $m = 2$. The second-order elastic coefficients were $c_{11} = 166$, $c_{12} = 64$, $c_{44} = 80$ GPa. The mentioned TOEC have been recalculated here onto equivalent ones that refer to the Biot and logarithmic strain measures, see rows 3 and 4. Additionally, in the last row the strain measure has been chosen in such a way to get a Hookean material for which the second-order bulk modulus vanishes.

Table 1. Third-order elastic coefficients [GPa] for silicon related to different strain measures.

m	$\widehat{C}_{111}$	$\widehat{C}_{112}$	$\widehat{C}_{123}$	$\widehat{C}_{144}$	$\widehat{C}_{155}$	$\widehat{C}_{456}$	$\partial\widehat{B}/\partial\hat{\varepsilon}$
2	−815	−450	−75	16	−307	−82	−1124
1	−317	−386	−75	48	−170	−22	−928
0	181	−322	-75	80	−32	38	−544
−2.155	1254	−184	−75	149	266	167	0

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