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AN APPROACH TO THE MATERIAL DEGRADATION

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An approach to the material degradation modeling is advanced in this paper on the base of the fabric tensors concept. Fabric tensors describe directional data like microcrack distributions and microstructural anisotropy in the material. Microcrack distributions within the material are used in the characterization and evaluation of damage. The damaged second- and third-order elastic constants for a caesium dihydrogen phosphate crystal are evaluated.

Key words: Damage mechanics, degradation, microcracks, fabric tensors, second- and third-order elastic constants.

1. INTRODUCTION

Damaged materials form a class of unusual elastic materials that show extreme nonlinearity, hysteresis and discrete memory. This class includes pearlitic steel, fiber-reinforced metal matrix composites, cement, concrete, ceramics, rocks, sand, soil etc. The bond systems consist of a fabric of defects (cracks, voids) that participates in the elastic response of the material. The grains have a random position and the intergranular interfaces contain cavities, microvoids, defects [1]. For most real materials the influences of the internal structure and the nature of the layer-like bonding are reflected not only in the values of the second-order elastic constants, but also in the values of higher-order elastic constants and particularly that of the third-order elastic constants [2]-[4]. These constants reflect the properties of materials. This paper is devoted to the analysis of the damage in materials, which are aggregates of grains which act as rigid vibrating units, while the contacts between them - the bond system - constitute a set of interfaces that control the behaviour of the material. At the mesoscopic scale, the micropolar continuum mechanics possesses a great potential to describe the long-range interactions among the particles in materials [5]-[7]. The interfaces are mesoscopic, with a typical size of 1 μm [8]-[9]. The theory of continuum damage mechanics was introduced in [10] for the isotropic case of uniaxial tension and later modified for creep in [11]. The damage variable is interpreted as the effective surface density of microdamages per unit volume. Kachanov has introduced the concept of effective stress, based on considering a fictitious undamaged configuration of a body and comparing it with the actual damaged configuration. The constitutive equations of evolution developed to predict the initiation of microcracks are basic on the damage variable [12]-[14].

The fabric tensors are introduced to model the damage mechanics by Voyiadjis and Kattan in 2005 [15]. Fabric tensors describe directional data like microcrack distributions and microstructural anisotropy in the material [16]. In this paper, the fabric tensors are used to characterize the damage in materials by describing the directional data and anisotropy. The proposed development is relevant for anisotropic materials, where inelastic deformations are accompanied by material degradation due to the evolution of microcracks. The degradation is measured by a decrease in the elastic constants values. As an example, the damaged second- and third-order elastic constants for a caesium dihydrogen phosphate crystal are evaluated.

2. THEORY

The idea of fabric tensors with regard to the distribution of directional data is introduced by Kanatani [17]. He used fabric tensors for the stereological determination of structural anisotropy. A distribution of microcracks that is radially symmetric with respect to the origin is considered here. Let us denote by $n^{(\alpha)}$, $\alpha = 1,...,M$, the unit vector specifying the orientation of the microcrack α , where M is the total number of microcracks. The orientation distribution function is denoted by $f(N)$, where the second-rank tensor N is defined as [17]

$$N_{ij} = \frac{1}{M}\sum_{\alpha=1}^{M} n_i^{(\alpha)} n_j^{(\alpha)} . \tag{2.1}$$

The function $f(N)$ can be then expanded in a convergent Fourier series as

$$f(N) = G^{(0)} + G_{ij}^{(1)} F_{ij}^{(1)}(N) + G_{ijkl}^{(2)} F_{ijkl}^{(2)}(N) + ..., \tag{2.2}$$

where $G^{(0)}$, $G_{ij}^{(1)}$, $G_{ijkl}^{(2)}$ are zero-rank (scalar), second-rank, and fourth-rank fabric tensors, respectively, and $F_{ij}^{1}(N)$, $F_{ijkl}^{2}(N)$ are zero-rank (scalar), second-rank, and fourth-rank basis functions, respectively. By denoting S , the surface of the unit sphere, the definition of fabric tensors is given by [18]-[20]

$$G^0 = \frac{1}{4\pi}\int_S f(N)\mathrm{d}A \, , \; G^1 = \frac{15}{8\pi}\int_S f(N)F^{(1)}(N)\mathrm{d}A \, , \; G^2 = \frac{315}{32\pi}\int_S f(N)F^{(2)}(N)\mathrm{d}A \, , \tag{2.2}$$

where A is the integration parameter. Only the first three terms in the expansion (2.2) are enough to describe material anisotropy. Therefore, we neglect the higher terms in the expansion and retain only the first three terms. The approximation of the distribution function $f(N)$ given in (2.2) characterizes anisotropy. The scalar $G^{(0)}$ describes the special case of isotropy, the tensor $G_{ij}^{(1)}$ describes orthotropy with three orthogonal planes of symmetry and all three eigenvalues being distinct. The case of transverse isotropy is characterized if the second-rank tensor $G_{ij}^{(1)}$ has only two distinct eigenvalues. The tensor $G_{ijkl}^{(2)}$ describes the materials with highest cubic symmetry and all kinds of anisotropy.

The second-order elastic constitutive relation for the damaged material is written in the actual damage state as [4]

$$\sigma_{kl} = C_{klmn}\varepsilon_{mn}(1-\varepsilon_{pp}) + C_{plmn}h_{kp}\varepsilon_{mn} + C_{kpmn}\varepsilon_{mn}h_{lp} + \frac{1}{2}C_{klmn}h_{pm}h_{pn} + \frac{1}{2}C_{klmnrs}\varepsilon_{mn}\varepsilon_{rs} \, , \tag{2.4}$$

where σ_{ij} is the stress tensor, $\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ is the strain tensor (the Lagrangian linear strain tensor), $h_{ij} = u_{i,j}$ the displacement gradient, C_{ijkl} is the second-order elastic constants of the damaged material and C_{ijklmn} is the third-order elastic constants of the damaged material. A similar elastic constitutive relation can be considered for a fictitious state of the material which is totally undamaged, i.e. all damage in this state has been removed. This fictitious state is assumed to be mechanically equivalent to the actual damaged state of the material, from the elastic strain equivalence or elastic energy equivalence point of view. By denoting $\bar{\sigma}_{ij}$ the effective stress tensor (the stress applied to a undamaged fictitious state of the material), $\bar{\varepsilon}_{ij}$ the effective strain tensor, $\bar{h}_{ij} = \bar{u}_{i,j}$ the effective displacement gradient, $\bar{C}_{jkl}$ the second-order elastic constants of the undamaged material and $\bar{C}_{ijklmn}$ the third-order elastic constants of the undamaged material, we can write

$$\bar{\sigma}_{kl} = \bar{C}_{klmn}\bar{\varepsilon}_{mn}(1-\bar{\varepsilon}_{pp}) + \bar{C}_{plmn}\bar{h}_{kp}\bar{\varepsilon}_{mn} + \bar{C}_{kpmn}\bar{\varepsilon}_{mn}\bar{h}_{lp} + \frac{1}{2}\bar{C}_{klmn}\bar{h}_{pm}\bar{h}_{pn} + \frac{1}{2}\bar{C}_{klmnrs}\bar{\varepsilon}_{mn}\bar{\varepsilon}_{rs} \, , \tag{2.5}$$

The pair tensors C_{ijkl}, $\bar{C}_{ijkl}$ and C_{ijklmn}, $\bar{C}_{ijklmn}$ can be related by the following relations

$$C_{ijkl} = (G^0 I_{mn} + G^{(1)}_{pq}) I_{ijkl} \bar{C}_{mnpq}\,,\ C_{ijklmn} = (G^0 I_{pq} + G^{(1)}_{rs} + G^{(2)}_{rsuv}) I_{ijklmn} \bar{C}_{pqrsuv}\,, \tag{2.6}$$

where I_{ijkl} and I_{ijklmn} are the unity tensors.

From (2.6) it results that the elastic strain tensor ε_{ij} and the displacement gradient h_{ij} in the actual damaged state, are related to the effective elastic strain tensor $\bar{\varepsilon}_{ij}$ and respectively, the effective displacement gradient $\bar{h}_{ij}$ in the fictitious state, by the laws

$$\bar{\varepsilon}_{ij} = I_{ijkl} f(N) \varepsilon_{kl}\,,\ \bar{h}_{ij} = I_{ijkl} f(N) h_{kl}\,, \tag{2.7}$$

where the function $f(N)$ is given by (2.2)

$$f(N) = G^{(0)} + G^{(1)}_{ij} F^{(1)}_{ij}(N).$$

By substituting (2.7) into (2.5), we obtain

$$\begin{aligned}\bar{\sigma}_{kl} &= \bar{C}_{klmn}\delta_{mnpq} f \varepsilon_{pq}(1-\delta_{ppqq} f \varepsilon_{qq}) + \bar{C}_{plmn}\delta_{kprs}\delta_{ijkl}\delta_{mnpq} f^3 h_{rs}\varepsilon_{pq} + \bar{C}_{kpmn}\delta_{mnpq}\delta_{lpuv} f^2 \varepsilon_{pql} h_{uv} + \\ &\frac{1}{2}\bar{C}_{klmn}\delta_{pmuv}\delta_{pnwt} f^2 h_{uv} h_{wt} + \frac{1}{2}\bar{C}_{klmnrs}\delta_{mnpq}\delta_{rsuv} f^2 \varepsilon_{pq}\varepsilon_{uv}\,,\end{aligned} \tag{2.8}$$

and by substituting (2.6) into (2.4), we have

$$\begin{aligned}\sigma_{kl} &= (G^0 I_{pq} + G^{(1)}_{rs}) I_{klmn} \bar{C}_{pqrs} \varepsilon_{mn}(1-\varepsilon_{pp}) + (G^0 I_{rs} + G^{(1)}_{uv}) I_{plmn} \bar{C}_{rsuv} h_{kp} \varepsilon_{mn} + \\ &(G^0 I_{uv} + G^{(1)}_{wt}) I_{kpmn} \bar{C}_{uvwt} \varepsilon_{mn} h_{lp} + \frac{1}{2}(G^0 I_{pq} + G^{(1)}_{uv}) I_{kllm} \bar{C}_{pquv} h_{pm} h_{pn} + \quad , \\ &\frac{1}{2}(G^0 I_{pq} + G^{(1)}_{uv} + G^{(2)}_{wt}) I_{klmnrs} \bar{C}_{pquvwt} \varepsilon_{mn}\varepsilon_{rs}\,.\end{aligned} \tag{2.9}$$

The equations (2.8) and (2.9) relate the actual state stress to the fictitious state stress. From this point, the specific strain energy functions U, $\bar{U}$ for damaged and undamaged material can be written from (2.7)-(2.9), respectively

$$\bar{U} = \frac{1}{2}\bar{\sigma}_{ij}\bar{\varepsilon}_{ij}\,. \tag{2.10}$$

From (2.10) we can obtain a scalar damage γ which relates the actual strain energy to the fictitious strain energy

$$U = \frac{\bar{U}}{1-\gamma}\,,\ \gamma \neq 1\,. \tag{2.11}$$

Damage development can be described by different values $\gamma < 1$, when $\gamma \to 1$. .`

3. THE CASE OF A MONOCLINIC CRYSTAL

The elastic behaviour of ferroelectric crystals is correlated with the microstructure and layer-like structure of the material [21] For a caesium dihydrogen phosphate lattice the damage due to the microcracks and microstructural anisotropy is reflected not only in the values of the second-order elastic constants but also in the values of higher-order elastic constants and particular that of the third-order elastic constants.

Consider a monoclinic crystal having a rectangular form of thickness h, length l and width d with respect to the Cartesian axes x_1, x_2, x_3. The Cartesian axes have a standard orientation with respect to the crystallographic axes a, b, c (fig.3.1). The axes a and c are perpendicular to b, but not to each other. The Cartezian coordinate system is located in the upper plane of the crystal with the x_3 axis normal to this plane. The origin point is the intersection of the diagonals, and the crystal edge is located at $x_2 = \pm l/2$ and $x_1 = \pm d/2$. The crystal contains a set of microcracks oriented in such a way that the normal to half of these microcracks has an angle θ = 90° while the normal to the other half has an angle θ = 0°. From (2.1) we obtain

$$N_{11} = N_{22} = \frac{1}{M}\sum_{\alpha=1}^{M}\left(\cos\theta^{(\alpha)}\right)^2 = \frac{1}{M}\left(\frac{M}{2}(\cos 0)^2 + \frac{M}{2}(\cos 90)^2\right) = \frac{1}{2},\ N_{33} = 0,\ N_{ij} = 0,\ i \neq j .$$

The values of undamaged elastic constants are found in [3]. The values of damaged elastic constants are calculated from (2.6).

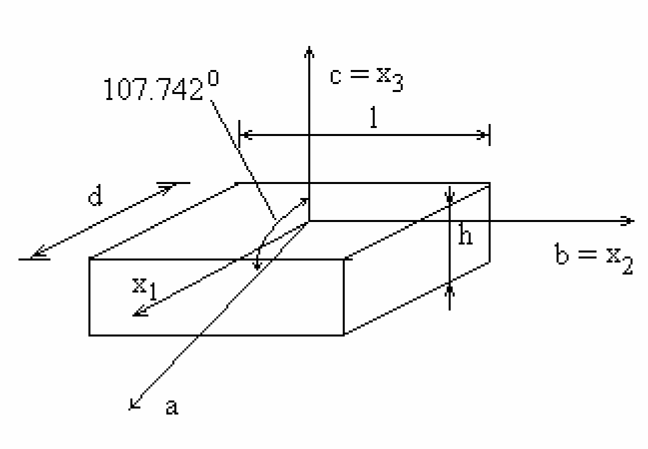

Fig.3.1. Axes of a monoclinic crystal.

In the monoclinic system we have 13 independent second-order elastic constants and 32 third-order elastic constants

$$C_{ijkl} = C_{\alpha\beta} = \left(C_{11}, C_{12}, C_{13}, C_{16}, C_{22}, C_{23}, C_{26}, C_{33}, C_{36}, C_{44}, C_{45}, C_{55}, C_{66}\right),$$

$$C_{ijklmn} = C_{\alpha\beta\gamma} = (C_{111}, C_{112}, C_{113}, C_{116}, C_{122}, C_{123}, C_{126}, C_{133}, C_{136}, C_{144}, C_{145}, C_{155}, C_{166}, C_{222}, C_{223},$$
$$C_{226}, C_{233}, C_{236}, C_{244}, C_{245}, C_{255}, C_{266}, C_{333}, C_{336}, C_{344}, C_{345}, C_{355}, C_{366}, C_{446}, C_{456}, C_{556}, C_{666})$$

with $\alpha = \beta = 1,2...6$.

Tables 3.1 and 3.2 show us the values of damaged elastic constants compared to the values of undamaged elastic constants. It is observed that the effect of the microcracks presence is a decreasing of the values for the second- and third-order elastic constants.

From tables, we see that the second-order elastic constants suffer a damage which is larger than the damage of the third-order elastic constants. The ratio between the undamaged and damaged values is about 1.4 for second-order elastic constants and about 1.32 for the third-order elastic constants. The value of the scalar damage γ is calculated from (2.11), and it is $\gamma = 0.277$. If introduce the constants ratios $C = \frac{\bar{C}}{1-\gamma}$, $\gamma \neq 1$, we obtain approximately $\gamma = 0.285$ for the second-order elastic constants, and $\gamma = 0.242$ for the third-order elastic constants. It results from here that (2.11) represents a measure for the elastic constants damage.

Table 3.1 The damaged second-order elastic constants compared to the undamaged elastic constants [3]

Elastic constant	Damaged values [GPa]	Undamaged values [GPa] Chiroiu *et al.*[3]	Elastic constant	Damaged values [GPa]	Undamaged values [GPa] Chiroiu *et al.*[3]
C_{11}	20.49	28.83	C_{26}	6.75	8.40
C_{12}	8.32	11.40	C_{33}	46.73	65.45
C_{13}	30.76	42.87	C_{36}	5.36	7.50
C_{16}	3.66	5.13	C_{44}	5.84	8.10
C_{22}	19.23	26.67	C_{45}	- 1.60	- 2.25
C_{23}	10.38	14.50	C_{55}	3.75	5.20

Table 3.2 The damaged third-order elastic constants compared to the undamaged elastic constants [3]

Elastic constant	Damaged values [GPa]	Undamaged values [GPa] Chiroiu *et al.*[3]	Elastic constant	Damaged values [GPa]	Undamaged values [GPa] Chiroiu *et al.*[3]
C_{111}	- 33.45	- 44.22	C_{233}	-9.44	-12.50
C_{112}	- 24.82	- 32.80	C_{236}	-9.87	-13.00
C_{113}	- 23.86	- 31.50	C_{244}	11.07	14.65
C_{116}	9.64	12.75	C_{245}	- 9.52	- 12.50
C_{122}	11.32	14.95	C_{255}	9.82	12.00
C_{123}	11.05	14.60	C_{266}	- 8.64	- 11.50
C_{126}	7.38	9.75	C_{333}	17.42	23.00
C_{133}	- 8.52	- 11.25	C_{336}	-9.55	-12.50
C_{136}	- 16.13	- 21.30	C_{344}	-17.41	-23.00
C_{144}	10.17	13.35	C_{345}	17.09	22.50
C_{145}	-6.61	-8.60	C_{355}	- 9.68	- 12.65
C_{155}	-7.35	-9.65	C_{366}	-10.22	-13.50
C_{166}	-23.86	-31.50	C_{446}	11.36	15.00
C_{222}	-11.02	-14.55	C_{456}	9.45	12.50
C_{223}	-7.23	-9.55	C_{556}	17.06	22.50
C_{226}	17.42	23.00	C_{666}	-10.23	-13.50

4. CONCLUSIONS

In this paper, the continuum damage mechanics is analysed through the concept of fabric tensors within the framework of nonlinear elasticity theory. A model of microcrack distributions data for the damaged materials is formulated by using fabric tensors. Fabric tensors describe microcrack distributions and microstructural anisotropy in the material. Microcrack distributions within the material are used in the characterization and evaluation of damage. The microstructure is related, through the use of fabric tensors, to the second-order and the third order elastic constants. As an example, the damaged second- and third-order elastic constants for a crystal of caesium dihydrogen phosphate are evaluated for a given set of microcracks.

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REFERENCES

1. CHIROIU, V., DUMITRIU, D., MITU, A.M., BALDOVIN, D., SECARA, C., *On the damage in nonlinear mesoscopic materials*, Proceeding of the European Computing Conference, Athens, Vouliagmeni Beach, Athens, Greece, September 25-27, Springer 2007.
2. CHIROIU, V., DELSANTO, P. P., MUNTEANU, L., RUGINA, C., SCALERANDI, M., *Determination from the natural frequencies of the second and third order elastic constants in Al*, Journal of the Acoustical Society of America, **102,** pp.193–198, 1997.
3. CHIROIU, C., MUNTEANU, L., CHIROIU, V., DELSANTO, P.P., SCALERANDI, M., *A genetic algorithm for determining of the elastic constants of a monoclinic crystal*, Inverse Problems **16**, pp.121-132, 2000**.**
4. TEODOSIU, C., *Elastic Models of Crystal Defects* (Berlin: Springer, Bucharest: Editura Academiei, 1982.
5. KACHANOV, L.M., *Time of the rupture process under creep conditions*, Izv. Akad., SSSR, Otd. Tech. Nauk., **8**, pp.26–31.
6. LEMAITRE, J., *A continuous damage mechanics model for ductile fracture*, ASME, J. Eng. Materials Technology, **107**, pp.83–89, 1985.
7. LEMAITRE, J., *Micromechanics of crack initiation*, Int. J. Fracture, **42**, pp.87–99, 1990.
8. GUYER, R.A., MCCALL, K.R., BOITNOTT, G.N., *Hysteresis, discrete memory, and nonlinear wave propagation in rock*, Phys.Rev.Lett., **74**, pp3491–3494, 1995.
9. GUYER, R.A., JOHNSON, P.A., *Nonlinear mesoscopic elasticity: Evidence for a new class of materials*, Physics Today, april, 1999.
10. KACHANOV, L., *On the Creep Fracture Time*, Izv Akad, Nauk USSR Otd Tech., **8**, pp. 26–31 (in Russian), 1958.
11. RABOTNOV, Yu., *Creep Rupture*, In Proceeding of the XII International Congress on Applied Mechanics, pp. 342–349, 1969.
12. LEMAITRE, J., *A Course on Damage Mechanics*, Second Edition, Springer-Verlag, New York, 1996.
13. CHABOCHE, J. L., *Une Loi Differentielle d'Endommagement de Fatigue avec Cumulation Non-lineare*, Rev. Francaise Mecanique, 50-51, 1974.
14. CHABOCHE, J. L., *Continuum Damage Mechanics: Present State and Future Trends*, International Seminar on Local Approach of Fracture, Moret- Sur-Loing, France, 1986.
15. VOYIADJIS, G. Z., KATTAN, P. I., *Damage Mechanics with Fabric Tensors*, Submitted for Publication, 2005.
16. Taqieddin, Ziad N., *Damage mechanics of composite materials using Fabric Tensors*, PhD thesis, Louisiana State Univ., 2005.
17. KANATANI, K., *Distribution of Directional Data and Fabric Tensors*, International Journal of Engineering Science, **22**, *2*, pp.149–164, 1984.
18. ZYSSET, P., CURNIER, S., *An Alternative Model for Anisotropic Elasticity Based on Fabric Tensors*, Mechanics of Materials, **21**, pp. 243–250, 1995.
19. ZYSSET, P., CURNIER, S., *A 3D Damage Model for Trabecular Bone Based on Fabric Tensors*, Journal of Biomechanics, **29**, *12*, pp.1549–1558, 1996.
20. CAUVIN, A., TESTA, R., *Damage Mechanics: Basic Variables in Continuum Theories*, International Journal of Solids and Structures, **36**, pp. 747–1761, 1999.
21. PRAWER, S., SMITH, T.F., FINLAYSON, T.R., *The room temperature elastic behaviour of CsH2PO4*, Australian Journal , 38, 1, 1985**.**

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