Journal of Theoretical and Applied Mechanics, Sofia, 2010, vol. 40, No. 4, pp. 41–54

SOLID MECHANICS

NEW APPROACH TO MODELLING THE DEFORMATIONAL PROCESSES IN CRYSTALLINE SOLID BODIES*

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[Received 05 October 2009. Accepted 04 October 2010]

Abstract. In the present paper some now-a-days approaches to modelling the deformation processes in the crystalline bulk materials are discussed: (i) multilevel models on macro and meso level; (ii) thermodynamic approach using EIT (Extended Irreversible Thermodynamic), especially for meso level; (iii) modern experimental methods; (iv) modern calculation methods.
Key words: multilevel model, crystalline body, experimental method.

1. Introduction

The deformation processes in crystalline bulk materials are taken into account. There are two different kinds of deformational processes in materials: during technological preparation of the material and during the exploitation of some devices like a structural material. Nevertheless, they are commune approaches in both cases. Some new approaches in design of the technology of material preparation or of the details of machines, structures, vehicles etc. will be discussed: (1) multilevel modelling taking into account the processes on a macro engineering level, meso structural level of the crystalline grains and a micro level presenting a micro structural object or defects. It is necessary to have information for a macro design about the micro-mechanisms of non-elastic macro-deformation, micro-defects, macro damage provoked and so on; (2) a proposition of appropriate process measures on the three levels.

*This part of the paper is supported by NF "Scientific research" under the grand No BYTH 211/2006 and it is precented like plenary lecture.

This gives the possibility to connect the processes on different levels and to have a good physical interpretation of the introduced measures; (3) We introduce not only the mechanical and structural measures taking into account the complexity of the processes, but also, in many cases, thermal, physical-chemical, electrical-magnetic measures and so on. This fact imposes to apply different thermodynamic schemes during multilevel modelling. The scheme of the Extended Irreversible Thermodynamics (EIT) is especially useful on meso structural level, because different fluxes may be introduced. These fluxes give a good interpretation about the development of the structural or defect changes; (4) Proposition of some experimental procedures giving information about the deformation processes on the three levels is derived. A numerical procedure will be presented to interpret the data from optical experimental methods in 2D; (5) Discussion about possibility in perspective to use a physical parallel numerical algorithm for deformational processes on macro and meso levels with an exchange of the information between them. This gives a useful realization of the macro design taking into account the process evolutions on both levels.

2. Multilevel modelling [2, 3, 7, 9, 14]

Isothermal mechanical-structural deformational processes in the bulk crystalline materials are regarded. It is needed to choose for modelling from the convenient measures and to propose adequate constitutive equations on the levels under consideration (macro and meso). The objects are discrete on micro level, but the continuum mechanics approach is very useful on macro and meso levels.

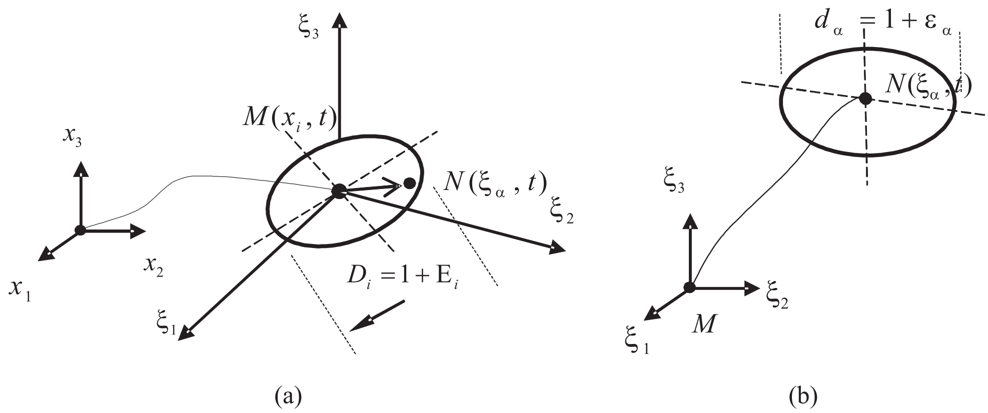

Fig. 1. The Representative Volume Element on (a) macro level and (b) meso level

A Representative Volume Element (RVE) is introduced on macro level as an ellipsoid at a body point M with Cartesian coordinates (x_1, x_2, x_3), (see Fig. 1) at a fixed moment $t \in [t_0, t_f]$, t_0 and t_f are the moments at the beginning and at the end of the process respectively.

The macro RVE-ellipsoid possesses principal diameters, $D_i = 1 + E_i$, $(i = I, II, III)$, where E_i are the principal macro strains. We introduce at point M the local co-ordinate system (M, ξ_1, ξ_2, ξ_3).

We introduce at point $N(\xi_1, \xi_2, \xi_3)$ a new meso RVE as an ellipsoid with principal diameters $d_i = 1 + \varepsilon_\alpha$, where ε_α, $(\alpha = 1, 2, 3)$ are the principal meso strains (see Fig. 1).

2.1. Model parameters

2.1.1. Macro level

The fallowing macro measures are taken into account.

Mechanical measures:

– macro stress tensor

$$\Sigma_{ij}, \quad (i, j = 1, 2, 3), \tag{2.1}$$

– macro strain tensor

$$E_{ij}, \quad (i, j = 1, 2, 3). \tag{2.2}$$

Structural measures:

– non-elastic residual macro strain tensor

$$E^p_{ij}. \tag{2.3}$$

Energetic measures:

U – Specific internal energy

S – Specific entropy

2.1.2. Meso level

Mechanical measures:

– meso stress tensor

$$\sigma_{\alpha\beta}, \quad (\alpha, \beta = 1, 2, 3), \tag{2.4}$$

– meso strain tensor

$$\varepsilon_{\alpha\beta}, \quad (\alpha, \beta = 1, 2, 3.) \tag{2.5}$$

Structural measures:

– meso residual strain tensor $\varepsilon^{p}_{\alpha\beta}$, arising from a system of m-structural tensor $g^{(q)}_{\alpha\beta}$ representing the micro defects on a meso level.

Representative structural defect tensors are:

$$g^{(q)}_{\alpha\beta} = \frac{1}{\upsilon_R}\int I^{(q)}_{\alpha\beta}\, d\upsilon \quad \text{is the mean measure of the } q\text{-defect,} \tag{2.6}$$

υ_R – volume of the Representative Volume Element (R.V.E.) on meso level.

The non-elastic strain tensor on meso level is:

$$\varepsilon^{(p)}_{\alpha\beta} = \sum_{q=1}^{m} L^{(q)}_{\alpha\beta\gamma\delta}\, g^{(q)}_{\gamma\delta}, \tag{2.7}$$

where $L^{(q)}_{\alpha\beta\gamma\delta}$ is the constitutive matrix of the q-defect.

The density of the q-defect:

$$\Pi^{(q)} = \sqrt{\frac{3}{2}\tilde{g}^{(q)}_{\alpha\beta}\,\tilde{g}^{(q)}_{\beta\alpha}}, \tag{2.8}$$

where $g^{(q)}_{\alpha\beta}$ is the deviator of the tensor $g^{(q)}_{\alpha\beta}$, $(q = 1, 2, \ldots, m)$.

We discretize the process with a small time interval Δt. The balance equation for the q-defect is:

$$\Delta\Pi^{(q)} = -J^{(q)}_{\alpha,\alpha} + \Delta\delta^{(q)}, \tag{2.9}$$

where $J^{(q)}_{\alpha}$ is the generalized flux vector of the q-defect. This is the definition equation for the vector $J^{(q)}_{\alpha}$.

Meso energetic measures:

u – Meso specific internal energy

s – Meso specific entropy

The following example concerning the plastic deformed materials will be given. We assume that the governing micro mechanism for the plastic deformation is the movement of the dislocation on activated shear planes e.g. $\alpha = 1$, and the tensor $g^{(1)}_{\alpha\beta}$ appears. The meso plastic strain tensor is $\varepsilon^{(p)}_{\alpha\beta} = \chi g^{(1)}_{\alpha\beta}$, where χ is the correlation coefficient. The movement of the dislocations is described by the flux vector $J^{(1)}_{\alpha}$ with the balance equation (2.9) for $\alpha = 1$. The value $\Delta\Pi^{(1)}$ is the density of the new dislocations initiated in the time interval Δt. The $\Delta\delta^{(1)}$ is the source of the new dislocations in Δt. This is a new look on the dislocation theory.

2.1.3. Micro level

Micro-structural measures of m-system of defects (dislocations, micro-cracks, micro-pores etc.):

$$I_{\alpha\beta}^{(q)}, \quad (q = 1, 2, \ldots, m), \tag{2.10}$$

$$I_{\alpha\beta}^{(q)} = S_{\alpha\beta}^{(q)} n_q \varphi_q, \quad S_{\alpha\beta}^{(q)} = \frac{1}{2}(n_\alpha^{(q)} m_\beta^{(q)} + n_\beta^{(q)} m_\alpha^{(q)}), \tag{2.11}$$

where $S_{\alpha\beta}^{(q)}$ is the Schmid tensor of orientation; n_q is the number of defects of type (q); φ_q is the specific reduction coefficient (see Fig. 2).

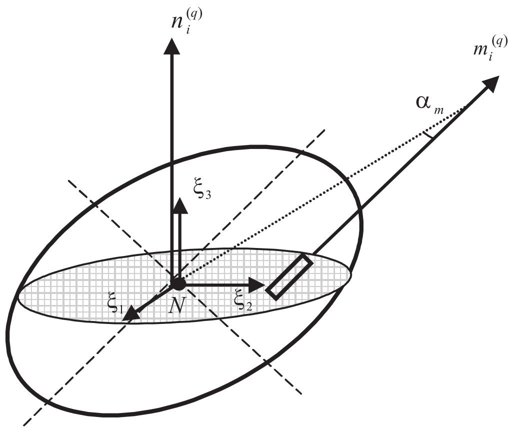

Fig. 2. Micro element in meso RVE

2.2. Constitutive relations [1, 6, 12, 15, 17]

We assume incremental constitutive relations for Δt-intervals, taking into account the elastic, plastic and damage properties.

2.2.1. Macro level

The following constitutive form is proposed on the basis of continuum mechanics

$$\Delta\Sigma_{ij} = H_{ijkl}\Delta E_{kl}, \quad \text{for} \quad \Delta t\text{-interval}, \tag{2.12}$$

where H_{ijkl} is the constitutive tensor depending on the total strain E_{ij} and non-elastic strain E_{ij}^p at the moment $t \in [t_0, t_I]$. The flow rule is assumed in the well-known form:

$$\Delta E_{ij}^p = \Delta\Lambda \frac{\partial F}{\partial \Sigma_{ij}}, \text{ for } F \geq 0, \tag{2.13}$$

where $\Delta\Lambda$ is the constitutive multiple; $F = 0$ is the non-elastic condition taken in the case of kinematics hardening:

$$F = F(\Sigma_{ij} - \Sigma^p_{ij}, E^p_{ij}), \quad (i, j = 1, 2, 3), \tag{2.14}$$

where Σ^p_{ij} is the plastic stress tensor thermodynamically coupled with E^p_{ij}, (see §3).

2.2.2. Meso level

We assume again the continuum mechanics scheme and the incremental constitutive form:

$$\Delta\sigma_{\alpha\beta} = h_{\alpha\beta\gamma\delta}\Delta\varepsilon_{\gamma\delta}, \quad \text{for} \quad \Delta t\text{-interval}, \tag{2.15}$$

where $h_{\alpha\beta\gamma\delta}$ is the constitutive tensor depending on $\varepsilon_{\alpha\beta}$ and $\varepsilon^p_{\alpha\beta}$ at moment t. The corresponding flow rule is the following:

$$\Delta\varepsilon^p_{\alpha\beta} = \Delta\lambda\frac{\partial f}{\partial\sigma_{\alpha\beta}}, \quad \text{for} \quad f \geq 0, \ (\alpha, \beta = 1, 2, 3), \tag{2.16}$$

with the constitutive multiple $\Delta\lambda$ and the non-elastic yield conditions:

$$f = f(\sigma_{ij}, \varepsilon^p_{ij}) = 0. \tag{2.17}$$

3. Thermodynamic scheme [2, 4, 5]

The thermodynamic scheme using Extended Irreversible Thermodynamics (EIT) is applied.

3.1. Macro level

We assume the existence of the function specific macro entropy:

$$S = S(U, E_{ij}; E^p_{ij}). \tag{3.18}$$

Variation of the entropy function during the time interval Δt is as follows:

$$\Delta U = \frac{1}{\rho}\Sigma_{ij}\Delta E_{ij}, \tag{3.19}$$

where ρ is the material density,

$$\Delta S = \frac{\partial S}{\partial U}\Delta U + \frac{\partial S}{\partial E_{ij}}\Delta E_{ij} + \frac{\partial S}{\partial E^a_{ij}}\Delta E^p_{ij}. \tag{3.20}$$

Thermodynamic conclusions on the basis of the First Thermodynamic Principle are in the well-known forms:

$$\Theta = \frac{\partial S}{\partial U}, \text{ macro temperature;} \quad \Theta = \Theta_0 = \text{const.}, \tag{3.21}$$

$$\rho \frac{\partial S}{\partial E_{ij}} = \Sigma_{ij}, \quad \rho \frac{\partial S}{\partial E^p_{ij}} = \Sigma^p_{ij},$$

where Σ^p_{ij} is the plastic stress tensor, as a generalized thermodynamic form.

The corresponding dissipation function in Δt-time interval becomes as follows:

$$\frac{1}{V_R}\Delta\Omega = \frac{1}{V_R}\Sigma^p_{ij}\, E^p_{ij} \geq 0, \; V_R \text{ is the volume of R.V.E.} \tag{3.22}$$

We assume the linearized relations in the time interval Δt:

$$\Delta\Sigma^p_{ij} = \Lambda^p_{ijkl}\,\Delta E^p_{kl}, \tag{3.23}$$

where the constitutive matrix $\{\Lambda^p_{ijkl}\}$ is assumed to be with a constant coefficient in the Δt interval.

3.2. Meso level

The application of EIT is especially suitable for modelling a meso level.

The specific meso entropy function is assumed as follows:

$$s = s(u, \varepsilon_{\alpha\beta}, \quad \pi^{(q)}, \quad \Delta J^{(q)}_\alpha). \tag{3.24}$$

The change of the entropy function during the time interval Δt appears in the form, cited below:

$$\Delta s = \frac{\partial s}{\partial u}\Delta u + \frac{\partial s}{\partial \varepsilon_{\alpha\beta}}\Delta\varepsilon_{\alpha\beta} + \sum_{q=1}^{m}\frac{\partial s}{\partial \pi^{(q)}}\Delta\pi^q + \sum_{q=1}^{m}\frac{\partial s}{\Delta J^{(q)}_\alpha}\,\Delta\left(\Delta J^{(q)}_\alpha\right), \tag{3.25}$$

where $\Delta u = \frac{1}{\rho^*}\sigma_{\alpha\beta}\Delta\varepsilon_{\alpha\beta}$; ρ^* – meso material density; $J^{(q)}_\alpha$ is the flux vector of the q-defect on meso level; $\Delta J^{(q)}_\alpha$ is the increment of this vector for the time interval Δt. We obtain the following relations applying the First Thermodynamic Principle:

$$\theta = \frac{\partial s}{\partial u}, \text{ meso temperature,} \quad \Theta = \text{const.}, \tag{3.26}$$

$$\rho^* \frac{\partial s}{\delta \varepsilon_{\alpha\beta}} = \sigma_{\alpha\beta}, \quad \frac{\partial s}{\partial \pi^{(q)}} = p^{(q)}, \quad (q = 1, 2, \ldots, m), \tag{3.27}$$

$$\frac{\partial s}{\partial \left(\Delta J_\alpha^{(q)}\right)} = Q_\alpha^{(q)}, \tag{3.28}$$

where $p^{(q)}$ and $Q_\alpha^{(q)}$ are the generalized dissipative thermodynamic forces. The simplified assumption $\Theta = \Theta_0$ is taken:

$$\frac{1}{\upsilon_R}\Delta\omega = \frac{1}{\upsilon_R}\sum_{q=1}^{m}\left(p^{(q)}\Delta\pi^{(q)} + Q_\alpha^{(q)}\Delta\left(\Delta J_\alpha^{(q)}\right)\right) \geq 0, \tag{3.29}$$

with

$$\rho^*\Delta\pi^{(q)} = l^{(q)}\Delta p^{(q)}, \quad (q = 1, 2, \ldots, m)\,; \quad \Delta Q_\alpha^{(q)} = \chi_{\alpha\beta}^{(q)}\Delta J_\beta^{(q)}, \tag{3.30}$$

where $l^{(q)}$ and $\chi_{\alpha\beta}^{(q)}$ are the material constant parameters in the Δt interval, and $\Delta\pi^{(q)}$ is the change of density for the q-objects.

4. Experimental method and numerical interpretation (test sample) [8, 11, 13 and 16]

Now-a-days there are some possibilities to collect different information about the material behaviour during the deformation processes on the three levels under consideration. The perspective may be the combination between standard macro experiments with an optical (SEM, TEM etc.), or an indentation with experimental procedures (macro, micro or nano- indenters). One important problem is how to interpret the experimental results to obtain the base for macro and meso constitutive modelling.

A 2D example will be presented in the case when the change of the point position of posed point set on the specimen surface is observed and registered optically during the deformation process. Additional information is needed about the volume changes on macro and meso levels in the Continuum Mechanics. We will propose a numerical procedure for the interpretation of the experimental measurements.

A thin plate, with thickness $h \ll 1$, loaded in its middle surface is taken into account. The material possesses elastic-plastic properties and the process is an isothermal and a quasi-static.

4.1. Macro level

The process is divided in Δt-intervals.

A set with a step in the upper surface is introduced using an appropriate experimental technique. At the moment t_0 the set point M possess the coordinates Δx_i, $x_{Mi}(p)$ on the surface of the plate, $p = 1, 2 \ldots n$, $i = 1, 2$ (see Fig. 3a).

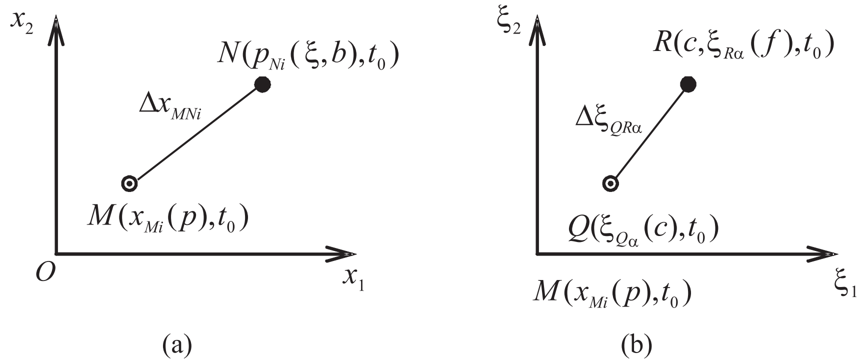

Fig. 3. Set points: (a) on macro level; (b) on meso level at the moment t_0

We choose the nearest point N $(x_{Ni}(b), t_0)$ in the neighborhood of point M, $b = 1, 2, 3$ with distances:

$$\Delta x_{MNi}(p, b, t_0) = x_{Ni}(\xi, b, t_0) - x_{Mi}(p, \xi, t_0)\,. \tag{4.31}$$

The new position of the point M at the moment $t_1 = t_0 + \Delta t$ is the point M' and for point N is point N'. The measured distance is:

$$\Delta x'_{MN}(p, b, t_1) = \Delta x'_M(p, b, t_1) - \Delta x'_N(p, b, t_1)\,, \tag{4.32}$$

and

$$\Delta U'_{Mi}(p, t_1) = x'_{Mi}(p, t_1) - x_{Mi}(p, t_0)\,, \tag{4.33}$$

$$\Delta U'_{Ni}(\xi, b, t_1) = x'_{Ni}(\xi, b, t_1) - x_{Ni}(\xi, b, t_0)\,. \tag{4.34}$$

The calculated unit vectors are:

$$n_{bi} = \frac{\Delta x_{Ni(b)}}{|\Delta x_{Ni}|} \quad \text{and} \quad n'_{bi} = \frac{\Delta x'_{Ni(b)}}{|\Delta x'_{Ni}|}. \tag{4.35}$$

The calculated strain E'_b in the direction n'_{bi} is:

$$E'_b(p,b,t_1) = E'_{11}(p,t_1)(n'_{b1})^2 + E'_{22}(p,t_1)(n'_{b2})^2 + \\ 2E'_{33}(p,t_1) + 2E'_{12}(p,t_1)(n'_{b1})(n'_{b2}) \,, \tag{4.36}$$

where $E'_{13} = 0$; $E'_{23} = 0$; $E'_{33} = \dfrac{h(t_1)}{h(t_0)}$.

The three linear equations system is formed for $b = 1,2,3$, and E'_{11}, E'_{22}, E'_{12} are defined.

The calculation procedure is again realized for moment t_2 and the derived difference is:

$$\Delta E''_{ij}(p,t_2) = E''_{ij}(p,t_2) - E'_{ij}(p,t_1), \tag{4.37}$$

with

$$\Delta E''_{33}(p,t_2) = \frac{h(t_2) - h(t_1)}{h(t_0)}. \tag{4.38}$$

The macro stresses at point M'' are calculated at moment t_2 using the equations of the equilibrium and the plastic incompressibility.

$$\frac{\delta\Sigma''_{11}(p,t_2)}{\delta x''_1} + \frac{\delta\Sigma''_{12}(p,t_2)}{\delta x''_2} = 0, \qquad \frac{\delta\Sigma''_{22}(p,t_2)}{\delta x''_2} + \frac{\delta\Sigma''_{12}(p,t_2)}{\delta x''_1} = 0, \tag{4.39}$$

where $\delta x''_i = x''_i(p_1,p_2) - x''_i(p-1,p_2)$ and

$$\frac{1}{3}\left(\Delta\Sigma''_{11}(p,t_2) + \Delta\Sigma''_{22}(p,t_2)\right) = K_e \Delta v'', \\ \delta\Sigma''_{ij} = \Delta\Sigma''_{ij}(p_1,t_2) - \Delta\Sigma''_{ij}(p-1,t_2) \tag{4.40}$$

where K_e is the volume elastic modulus, which is possible to derive experimentally.

$$\Delta\Sigma''_{13} = 0; \quad \Delta\Sigma''_{23} = 0; \quad \Delta\Sigma''_{33} = 0, \quad \text{plane stress state.} \tag{4.41}$$

The constitutive matrix $\{H_{ij}\}$, $(i,j = 1,2)$ is calculated using the following incremental relations:

$$\Delta E''_{11} = H''_{11}\Delta\Sigma''_{11} + H''_{12}\Delta\Sigma''_{12}, \tag{4.42}$$

$$\Delta E''_{22} = H''_{22}\Delta\Sigma''_{22} + H''_{21}\Delta\Sigma''_{21}, \tag{4.43}$$

$$\Delta E''_{12} = 2H''_{12}\Delta\Sigma''_{12} \quad \text{with} \quad H''_{12} = H''_{21}. \tag{4.44}$$

The constitutive matrix function will be obtained realizing the calculation procedure at the ξ number of moment t:

$$H_{ij} = \Phi_{ij}\left(E_{ke}\left(t\right), E^{p}_{ke}\left(t\right)\right), \tag{4.45}$$

where $E_{ij}\left(t\right)$ and $E^{p}_{ij}\left(t\right)$ are measured for every discreet moment t.

4.2. Meso level

We introduce a meso set with different steps $\Delta\xi_{\alpha}$ in the meso level R.V.E. at point M, where ξ_{α} is the co-ordinate of the middle surface of the plate. At the moment t_0 in the set point M possess the co-ordinates x_{Mi}.

The new set is introduced with a characteristic point Q (see Fig. 3b) is presented below:

$$Q\left(x_{Mi}\left(P\right); \xi_{Q\alpha}\left(c\right), t_0\right), \quad c = 1, 2\ldots, r;\ \rho = 1, 2\ldots n;\ i = 1, 2;\ \alpha = 1, 2. \tag{4.46}$$

Point $R\left(c, \xi_{R\alpha}\left(f\right), t_0\right)$ the nearest to point $Q\left(\xi_{Q\alpha}\left(c\right), t_0\right)$, $c = 1, 2, \ldots r$; $f = 1, 2, 3$; $\alpha = 1, 2$ is taken into account.

The calculated distance is:

$$\Delta\xi^{0}_{QR\alpha}\left(c, f, t_0\right) = \xi^{0}_{R\alpha}\left(c, f, t_0\right) - \xi^{0}_{Q\alpha}\left(c, t_0\right) \quad \text{at the moment} \quad t_0. \tag{4.47}$$

The measured new distance at the moment t_1 is:

$$\Delta\xi'_{QR\alpha}(c, f, t_1) = \xi'_{R\alpha}(\xi, f, t_1) - \xi'_{Q\alpha}(c, t_1), \tag{4.48}$$

and

$$\Delta u'_{Q\alpha}(c, t_1) = \xi'_{Q\alpha}(c, t_1) - \xi^{0}_{Q\alpha}(c, t_0), \tag{4.49}$$

$$\Delta u'_{R\alpha}(\xi, f, t_1) = \xi'_{R\alpha}(\xi, f, t_1) - \xi^{0}_{R\alpha}(\xi, f, t_0). \tag{4.50}$$

The strain ε'_c in the direction $n'_{f\alpha}$ is:

$$\begin{gathered} \varepsilon'_c(c, f, t_1) = \varepsilon'_{11}(c, t_1)(n'_{f1})^2 + \varepsilon'_{22}(c, t_1)(n'_{f2})^2 + 2\varepsilon'_{33}(c, t_1) + \\ 2\varepsilon'_{12}(c, t_1)(n'_{f1})(n'_{f2}) \end{gathered}, \tag{4.51}$$

where $\varepsilon'_{13} = 0$; $\varepsilon'_{23} = 0$; $\varepsilon'_{33} = E'_{33}$ (additional assumption).

At the moment t_2:

(4.52) $\Delta\varepsilon''_{\alpha\beta}(c,t_2) = \varepsilon''_{\alpha\beta}(c,t_2) - \varepsilon'_{\alpha\beta}(c,t_1)$ with assumption $\Delta\varepsilon''_{33} = \Delta E''_{33}$.

At the moment t_2 at point Q'':

(4.53) $$\frac{\delta\sigma''_{11}(c,t_2)}{\delta\xi''_1} + \frac{\delta\sigma''_{12}(c,t_2)}{\delta\xi''_2} = 0, \quad \delta\sigma''_{\alpha\beta}(c,t_2) = \varepsilon''_{\alpha\beta}(c,t_2) - \Delta\sigma'_{\alpha\beta}(c-1,t_2)$$

(4.54) $$\frac{\delta\sigma''_{22}(c,t_2)}{\delta\xi''_2} + \frac{\delta\sigma''_{12}(c,t_2)}{\delta\xi''_1} = 0, \quad \delta\xi''_{\alpha}(c,t_2) = \xi''_{\alpha}(c,t_2) - \Delta\xi''_{\alpha}(c-1,t_2)$$

and

(4.55) $$\frac{1}{3}\left(\Delta\sigma''_{11}(c,t_2) + \Delta\sigma''_{22}(c,t_2)\right) = k_e\Delta v'',$$

where $\Delta v'' = \Delta\varepsilon''_{11} + \Delta\varepsilon''_{22} + \Delta\varepsilon''_{33}$; $\Delta\varepsilon''_{33} = \Delta E''_{33}$ (assumption) k_e is the meso volume elastic modulus.

If we assume the constitutive model for the composite material [6, 9], for the two components (A) and (B) , $K_e(A) = K_e/v_A$, where v_A is the volume fracture of the component (A):

(4.56) $$\Delta\sigma''_{13} = 0; \quad \Delta\sigma''_{23} = 0; \quad \Delta\sigma''_{33} = 0, \text{ planestressstate},$$

for the meso constitutive matrix $\{h_{\alpha\beta}\}$, $(\alpha, \beta = 1, 2)$ it is calculated:

(4.57) $$\Delta\varepsilon''_{11} = h''_{11}\Delta\sigma''_{11} + h''_{12}\Delta\sigma''_{12},$$

(4.58) $$\Delta\sigma''_{22} = h''_{22}\Delta\sigma''_{22} + h''_{21}\Delta\sigma''_{21},$$

(4.59) $$\Delta\varepsilon''_{12} = 2h''_{12}\Delta\sigma''_{12}, \quad \text{with} \quad h''_{12} = h''_{21}.$$

We will obtain the constitutive matrix function on the meso level for a number of the moment t:

(4.60) $$h_{\alpha\beta} = \varphi_{\alpha\beta}\left(\varepsilon_{\gamma\delta}(t), \varepsilon^p_{\gamma\delta}(t)\right),$$

where $\varepsilon_{\gamma\delta}(t)$ and $\varepsilon^p_{\gamma\delta}(t) = \sum_{q=1}^{m} L^{(q)}_{\alpha\beta\gamma\delta} g^{(q)}_{\gamma\delta}(t)$ are measured for every discreet moment t.

5. Conclusions and perspectives

The main problem in 3D-modelling is the identifications of the structural or defects measures.

The application of the flux thermodynamic conception needs future development.

We propose like a perspective to use the physical parallel algorithm for both processes on macro and meso level. They must exchange the information during the calculation between the two levels.

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Presented at the 11th National Congress on Theoretical and Applied Mechanics, Borovets, Bulgaria, 2–5 September, 2009