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Constitutive Equations of the Nonlinear Crystal Lattice

Nonlinear deformation of ideal crystal lattice is investigated. Macroscopic stress tensors and dynamic equations are obtained from the microscopic dynamic equations. Microscopic interpretation for different stress tensors is given. This approach allows to show obviously correlation between the different stress tensors which are usually used in nonlinear theory of elasticity. Constitutive equations for nonlinear deformation of the crystal lattice are obtained. Approximations corresponding to the geometrical nonlinear material and Seth material are considered.

1 Introduction

One of the most complicated problems in nonlinear theory of elasticity is problem of construction of constitutive equations. That is why we use the simple mechanical model such as ideal monocrystal to obtain and investigate nonlinear constitutive equations. Let us use set of particles with potential central forces that form an ideal simple 3D crystal lattice. For each particle a limited number of neighbors is accepted. The forces and deformations are nonlinear. To obtain macroscopic equations from microscopic long wave approximation will be used.

Let us use the following designations. For the reference configuration $\underline{r}$ is radius vector, $\underline{a}_\alpha$ is radius vector of a node α from the current node, v_* is volume of elementary cell, $\overset{\circ}{\nabla}$ is nabla operator. For the actual configuration the corresponding quantities are $\underline{R}$, $\underline{A}_\alpha$, V_*, ∇. The nodes numbering uses the relation $\underline{a}_{-\alpha} \overset{def}{=} -\underline{a}_\alpha$.

2 Long wave approximation

The equation of equilibrium of a particle is $\sum\limits_\alpha \underline{F}_\alpha + \underline{f} = 0 \Leftrightarrow \frac{1}{2}\sum\limits_\alpha (\underline{F}_\alpha + \underline{F}_{-\alpha}) + \underline{f} = 0$, where $\underline{F}_\alpha$ is force acting from the particle α to the current particle, $\underline{f}$ is external force. In the *material representation*: $\underline{F}_\alpha = \underline{F}_\alpha(\underline{r})$. Then $\underline{F}_{-\alpha}(\underline{r})$ can be represented as $\underline{F}_{-\alpha}(\underline{r}) = -\underline{F}_\alpha(\underline{r} - \underline{a}_\alpha) \approx -\underline{F}_\alpha(\underline{r}) + \underline{a}_\alpha \cdot \overset{\circ}{\nabla} \underline{F}_\alpha(\underline{r})$, and the equation of equilibrium takes the form $\overset{\circ}{\nabla} \cdot \frac{1}{2}\sum\limits_\alpha \underline{a}_\alpha \underline{F}_\alpha + \underline{f} = 0$, which can be rewritten as macroscopic equation of equilibrium in Piola form

$$\overset{\circ}{\nabla} \cdot \underline{\underline{P}} + \rho_0 \underline{k} = 0\,; \qquad \underline{\underline{P}} \overset{def}{=} \frac{1}{2v_*}\sum_\alpha \underline{a}_\alpha \underline{F}_\alpha\,, \qquad \rho_0 \overset{def}{=} \frac{m}{v_*}\,, \qquad \underline{k} \overset{def}{=} \frac{1}{m}\underline{f}\,. \tag{1}$$

The *space representation*: $\underline{F}_\alpha = \underline{F}_\alpha(\underline{R})$ gives the macroscopic equation of equilibrium in Cauchy form

$$\nabla \cdot \underline{\underline{T}} + \rho \underline{k} = 0\,; \qquad \underline{\underline{T}} \overset{def}{=} \frac{1}{2V_*}\sum_\alpha \underline{A}_\alpha \underline{F}_\alpha\,, \qquad \rho \overset{def}{=} \frac{m}{V_*}\,. \tag{2}$$

3 Microscopic representation of macroscopic stress tensors

Using designation $\underline{F}_\alpha = \Phi_\alpha \underline{A}_\alpha$ from (1) and (2) we can obtain the following microscopic representation of macroscopic stress tensors frequently used in literature [1]

$$\underline{\underline{T}} = \frac{1}{2V_*}\sum_\alpha \Phi_\alpha \underline{A}_\alpha \underline{A}_\alpha \quad \text{Cauchy tensor}\,, \qquad \underline{\underline{\tilde{T}}} = \frac{1}{2V_*}\sum_\alpha \Phi_\alpha \underline{a}_\alpha \underline{a}_\alpha \quad \text{Energy tensor}\,,$$

$$\underline{\underline{T}}_{(o)} = \frac{1}{2v_*}\sum_\alpha \Phi_\alpha \underline{A}_\alpha \underline{A}_\alpha \quad \text{(Hamel)}\,, \qquad \underline{\underline{T}}^* = \frac{1}{2v_*}\sum_\alpha \Phi_\alpha \underline{a}_\alpha \underline{a}_\alpha \quad \text{2nd Piola tensor}\,,$$

$$\underline{\underline{P}} = \frac{1}{2v_*}\sum_\alpha \Phi_\alpha \underline{a}_\alpha \underline{A}_\alpha \quad \text{Piola tensor}\,, \qquad \underline{\underline{\Phi}} = \frac{1}{2}\sum_\alpha \Phi_\alpha \underline{a}_\alpha \underline{a}_\alpha \quad \text{Force tensor}\,.$$

The last tensor named "Force tensor" is introduced in this paper. Using it the constitutive equations of the nonlinear crystal lattice can be written in the form

$$\underline{\underline{T}} = \frac{1}{v_* |\underline{\underline{G}}|^{1/2}} (\underline{R}\overset{\circ}{\nabla}) \cdot \underline{\underline{\Phi}}(\underline{\underline{G}}) \cdot (\overset{\circ}{\nabla}\underline{R})\,, \qquad \underline{\underline{\Phi}}(\underline{\underline{G}}) = \frac{1}{2}\sum_\alpha \Phi(\underline{a}_\alpha \cdot \underline{\underline{G}} \cdot \underline{a}_\alpha)\, \underline{a}_\alpha \underline{a}_\alpha\,; \qquad \underline{\underline{G}} = (\overset{\circ}{\nabla}\underline{R}) \cdot (\underline{R}\overset{\circ}{\nabla})\,. \tag{3}$$

Here the function $\Phi(\underline{a}_\alpha \cdot \underline{\underline{G}} \cdot \underline{a}_\alpha) = \Phi(\underline{A}_\alpha \cdot \underline{A}_\alpha)$ is known microscopic relation.

4 Linear approximation

The general form of the constitutive equation (3) is very complex, so let us consider different approximations. The simplest of them is linear approximation:

$$\underline{A}_\alpha = \underline{a}_\alpha + \underline{\Delta}_\alpha\,, \qquad \underline{\Delta}_\alpha = \underline{u}(\underline{r} + \underline{a}_\alpha) - \underline{u}(\underline{r})\,, \qquad \underline{u} = \underline{R} - \underline{r}\,; \qquad |\underline{\Delta}_\alpha| \ll |\underline{a}_\alpha|\,, \qquad |\underline{a}_\alpha| \ll |\underline{r}|\,.$$

Expansion of constitutive equation (3) to power series in $\underline{\Delta}_\alpha$, $\underline{a}_\alpha$ gives

$$\underline{\underline{\tau}} = {}^4\underline{\underline{C}} \cdot\cdot\, \underline{\underline{\varepsilon}}\,, \qquad {}^4\underline{\underline{C}} = \frac{1}{v_*}\,{}^4\underline{\underline{B}} = \frac{1}{2v_*} \sum_\alpha B_\alpha \underline{a}_\alpha \underline{a}_\alpha \underline{a}_\alpha \underline{a}_\alpha\,, \qquad \underline{\underline{\varepsilon}} = (\nabla \underline{u})^s\,, \tag{4}$$

where $\underline{\underline{\tau}}$ is linear stress tensor, $B_\alpha \overset{def}{=} 2\Phi'(a_\alpha^2)$. In the case of isotropy the equation (4) can be written in the form

$$\underline{\underline{\tau}} = C\Big((\mathrm{tr}\underline{\underline{\varepsilon}})\underline{\underline{E}} + 2\underline{\underline{\varepsilon}}\Big)\,, \qquad C = \frac{1}{30} \sum_\alpha a_\alpha B_\alpha\,,$$

which corresponds to the Poisson coefficient: $\nu = 1/4$ — the known feature of the simple crystal lattice.

5 Geometrically nonlinear material

Let us consider material with linear forces of interaction, but nonlinear deformations. The force tensor in this case takes the form $\underline{\underline{\Phi}} = {}^4\underline{\underline{B}} \cdot\cdot\, \underline{\underline{\varepsilon}}$, where ${}^4\underline{\underline{B}}$ is defined by (4), $\underline{\underline{\varepsilon}} = \frac{1}{2}\,(\underline{\underline{G}} - \underline{\underline{E}})$ is Cauchy-Green tensor of finite deformation. Hence the constitutive equation (3) for geometrically nonlinear material reduces to

$$\underline{\underline{T}} = |\underline{\underline{G}}|^{-1/2} (\underline{R} \overset{\circ}{\nabla}) \cdot ({}^4\underline{\underline{C}} \cdot\cdot\, \underline{\underline{\varepsilon}}) \cdot (\overset{\circ}{\nabla} \underline{R})\,, \qquad {}^4\underline{\underline{C}} = \frac{1}{2v_*} \sum_\alpha B_\alpha \underline{a}_\alpha \underline{a}_\alpha \underline{a}_\alpha \underline{a}_\alpha\,. \tag{5}$$

Alternate forms with nonconstant tensor of stiffness can be used

$$\underline{\underline{T}} = {}^4\underline{\underline{C}}' \cdot\cdot\, \underline{\underline{\varepsilon}} = {}^4\underline{\underline{C}}'' \cdot\cdot\, \underline{\underline{\varepsilon}}'\,, \qquad {}^4\underline{\underline{C}}' \overset{def}{=} \frac{1}{2V_*} \sum_\alpha B_\alpha \underline{A}_\alpha \underline{A}_\alpha \underline{a}_\alpha \underline{a}_\alpha\,, \qquad {}^4\underline{\underline{C}}'' \overset{def}{=} \frac{1}{2V_*} \sum_\alpha B_\alpha \underline{A}_\alpha \underline{A}_\alpha \underline{A}_\alpha \underline{A}_\alpha\,. \tag{6}$$

Were $\underline{\underline{\varepsilon}}' = \frac{1}{2}\,(\underline{\underline{g}} - \underline{\underline{E}})$ is Almansi tensor of finite deformation, $\underline{\underline{g}} = (\nabla \underline{r}) \cdot (\underline{r} \nabla)$. In the case of isotropy

$$\underline{\underline{T}} = C|\underline{\underline{F}}|^{-1/2} \underline{\underline{F}} \cdot \Big((\mathrm{tr}\underline{\underline{\varphi}})\underline{\underline{E}} + 2\underline{\underline{\varphi}}\Big)\,, \qquad \underline{\underline{F}} = (\underline{R} \overset{\circ}{\nabla}) \cdot (\overset{\circ}{\nabla} \underline{R}) = \underline{\underline{Q}}^T \cdot \underline{\underline{G}} \cdot \underline{\underline{Q}}\,, \qquad \underline{\underline{\varphi}} = \frac{1}{2}\,(\underline{\underline{F}} - \underline{\underline{E}}) = \underline{\underline{Q}}^T \cdot \underline{\underline{\varepsilon}} \cdot \underline{\underline{Q}}\,.$$

Here the polar decomposition is used: $\overset{\circ}{\nabla} \underline{R} = \underline{\underline{U}} \cdot \underline{\underline{Q}}$, where $\underline{\underline{Q}}$ is tensor of turn, $\underline{\underline{U}}^2 = \underline{\underline{G}}$ [1]. If we consider small deformations, but displacements and turns are finite, then $\overset{\circ}{\nabla} \underline{R} \approx \underline{\underline{Q}}$ and the equation (5) takes the form: $\underline{\underline{T}} = \underline{\underline{Q}}^T \cdot ({}^4\underline{\underline{C}} \cdot\cdot\, \underline{\underline{\varepsilon}}) \cdot \underline{\underline{Q}}$. For isotropic case we obtain the constitutive equation of Seth material

$$\underline{\underline{\tau}} = C\Big((\mathrm{tr}\underline{\underline{\varepsilon}}')\underline{\underline{E}} + 2\underline{\underline{\varepsilon}}'\Big)\,; \qquad \underline{\underline{\varepsilon}}' = \underline{\underline{Q}}^T \cdot \underline{\underline{\varepsilon}} \cdot \underline{\underline{Q}}\,, \qquad \mathrm{tr}\,\underline{\underline{\varepsilon}}' = \mathrm{tr}\,\underline{\underline{\varepsilon}}\,.$$

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