Corotational derivatives in the numerical simulation of shock loading of deformable solid on the example of aluminum alloy 2024

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Abstract. The peculiarities of the use of the Jaumann and Green-Naghdi corotational derivatives were investigated for modeling deformation processes in isotropic and anisotropic materials under shock loading. Using the aluminum alloy 2024 as an example, it has been shown that taking into account the anisotropy of mechanical properties affects the values of the Jaumann and Green-Naghdi corotational derivatives upon returning the alloy to an unstressed state. It was proposed to use the combination of the Jaumann and Green-Naghdi corotational derivatives to increase the accuracy in numerical calculations of the stress tensor components.

1. Introduction

The rates of change of scalar and tensor quantities in time are determined in the numerical simulation of shock loading of solids (for example, by the finite element method). Direct use of the stress tensor components in the equations leads to incorrect results due to the rotation of the elements as a rigid whole. In particular, if relevant material line rotations occur, unreasonable phenomena, like stress oscillation in simple shear, dissipation in elastic strain cycles etc., may occur [1,2]. The method of getting rid of this defect is the use of corotational derivatives.

In the continuum mechanics, the corotational derivatives determine the rate of change of the tensors with respect to a certain mobile basis, i.e. relative velocities. They determine the rate of change in the values of the components of the tensor for an observer moving along with the chosen basis. This basis is immovable for the observer and therefore it does not differentiate by time.

Choosing different mobile bases, and on their basis calculating the corresponding spins, different corotational derivatives are obtained, each of which has its own characteristics in the implementation, and some of which has disadvantages.

Two derivatives are considered in this paper: the widely used Jaumann corotational derivative [2,3,4,5] and the Green-Naghdi derivative [6,7], which is rare in the literature

\[ \sigma^J = \dot{\sigma} - \omega \sigma + \sigma \omega \left( \omega = \frac{1}{2} \text{rot}\vec{v} \right) \]

\[ \sigma^G = \dot{\sigma} - \Omega \sigma + \sigma \Omega \left( \Omega = R R^T \right) \] (1)

where \( \omega \) - vortex tensor, \( \Omega \) - antisymmetric tensor of relative spin. \( R \) - orthogonal rotation tensor accompanying deformation. It is calculated from the polar expansion of the strain gradient tensor \( F \) \((F = R \cdot U = V \cdot R, U \) - right-distortion tensor, and \( V \) - left-distortion tensor) or through a combination...
of three rotation matrices relative to each axis of the basis by the corresponding angle (angles of Euler).

In the formal mathematical analysis of stresses, the use of these two derivatives has no advantages. However, in the numerical solution of the problems of the mechanics of a deformable solid, it is desirable to use the derivative that leads to a more accurate determination of the stress tensor components.

The value of the residual stresses arising after the first and subsequent cycles of loading of polycrystalline is investigated because of the errors introduced by these corotational derivatives [1]. This is especially important for modeling multiple cyclic loading of structural elements. Residual stresses after each cycle of loading may have a different negative effect on the final picture of the stress state when describing elastoplastic deformations in solids. Studies are carried out on the basis of consideration only of cyclic elastic deformation, which allows us to return to the unloaded state of solids.

When modeling the shock loading of solids, the wave pattern of deformation is characterized by the passage of two or three compression and stretching waves along the structural element, the passage of subsequent waves, as a rule, does not add to the process of deformation.

The cyclic stress in polycrystalline 2024 is considered within the framework of the hypotheses of bulk isotropy and bulk anisotropy of deformation processes, i.e. when modeling isotropic or anisotropic pressure in a material.

2. Basic Relationships
Stresses are considered as Kirchhoff stresses $\tau$, related to the Cauchy tensor or true stress $\sigma$ by the following relation

$$\tau = (\det F)\sigma \quad (3)$$

where $F$ - strain gradient tensor.

$$F = \frac{\partial x}{\partial X}, \det F > 0 \quad (4)$$

$X$ is the position of the material particle in the control configuration, and $x$ is the position in the current configuration.

It is necessary to decompose the tensors of total stresses and total deformations into parts related to the change in volume and shape when modeling elastoplastic deformations

$$\sigma_{ij} = -P\delta_{ij} + S_{ij} \quad (5)$$

$$E_{ij} = E_0\delta_{ij} + e_{ij}$$

The change in the form of the corotational derivative is due to the mismatch of a uniform stress state to a uniform deformed one for anisotropic solids.

To relate stresses and deformations in the general case of anisotropy, we use the generalized Hooke's law

$$\sigma_{ijkl} = c_{ijkl} e_{kl}, \quad i, j, k, l = 1, 2, 3 \quad (6)$$

where $c_{ijkl}$ - elastic constants forming a fourth-rank tensor.

If a uniform volume deformation is realized in a ball made of an anisotropic material, i.e. the ball under loading will retain the shape of the ball, then inside it will be realized a stress state having different values in the direction of its axes. This is due to the different values of the volumetric compressibility in anisotropic materials. In the case where an orbital hydrostatic pressure acts on a ball made of an anisotropic material, its shape changes, and it acquires the shape of an ellipsoid because of the different values of the volume compressibility along different axes. This reaction of the ball to loading is realized under static loads. This is one of the main features of the deformation of anisotropic materials.

For the isotropic case, the stress tensor is written uniquely $\sigma_{ij} = -P\delta_{ij} + S_{ij}$, where $\delta_{ij}$ - Kronecker symbols, and the componentwise representation of the derivatives (1) and (2) can be written only for the components of the stress deviator [3].
In the case of anisotropy of the elastic and plastic properties of a solid, the stress tensor is written differently [8]

\[
\sigma_{ij} = -P \lambda_{ij} + S_{ij}
\]  

(8)

where \( \lambda_{ij} \) - coefficients that depend on the elastic properties of the material (\( \lambda_{ij} \neq 0 \) for \( i = j \)). The componentwise record (1) and (2) taking into account (8) takes the following form

\[
\frac{d\sigma_{ij}}{dt} = \frac{dS_{ij}}{dt} - \lambda_{ij} \frac{dp}{dt} - \omega_{ik} S_{kj} + S_{ik} \omega_{kj} + P \omega_{ij} (\lambda_{jj} - \lambda_{ii})
\]

\[
\frac{d\sigma_{ij}}{dt} = \frac{dS_{ij}}{dt} - \lambda_{ij} \frac{dp}{dt} - \Omega_{ik} S_{kj} + S_{ik} \Omega_{kj} + P \Omega_{ij} (\lambda_{jj} - \lambda_{ii})
\]  

(9)

Comparing (7) and (9) one can see the differences that are present for isotropic and anisotropic media.

For example, for a single crystal of zinc, with allowance for its anisotropy, these terms can be from 25 to 80% of the terms associated with isotropic properties [9].

**Table 1.** Anisotropic characteristics \( \lambda_{ij} \) of single crystal of zinc.

| \( \lambda_{11} \) | \( \lambda_{22} \) | \( \lambda_{33} \) |
|-------------------|-------------------|-------------------|
| 0.742             | 1.129             | 1.129             |

These estimates will be somewhat smaller because of less pronounced anisotropic properties for polycrystals.

**Table 2.** Anisotropic characteristics \( \lambda_{ij} \) of alloy 2024.

| \( \lambda_{11} \) | \( \lambda_{22} \) | \( \lambda_{33} \) |
|-------------------|-------------------|-------------------|
| 0.9748            | 1.0126            | 1.0126            |

3. Cyclic loading

Consider a square element of size \( H \cdot H \) in Fig. 1, which is embedded in the Cartesian frame of reference \( X_i \). We impose a cyclic deformation in which both upper corners rotate in a circle with a radius \( r_{lim} \). The value of the radius \( r \) for 2024 is determined in such a way that during loading the material always remains within the framework of elastic deformations. The element is represented by
a combination of stretching\compression in the $X_2$ direction and shifting in the $X_1$ direction and remains in shape of a parallelogram. Deformation in the direction of $X_3$ is not superimposed. The square element returns to its original form at the end of the cycle. The deformation of an element in an actual configuration is described by the following

$$x_1 = X_1 + \frac{\sin \varphi}{1 + (1 - \cos \varphi)} X_2$$

$$x_2 = \left(1 + \frac{1 - \cos \varphi}{\frac{\varphi}{2}} \right) X_2$$

$$x_3 = X_3$$  \hspace{1cm} (10)

Applying (4) to (5) and using the relation (3) for stresses, taking into account (1) and (2), it is possible to obtain differential equations for changes of each stress component and, consequently, to perform numerical integration.

The normal Kirchhoff stresses $\tau_{11}$ and $\tau_{22}$ for the corotational derivatives Jaumann and Green-Naghdi is shown on Fig. 2. It can be seen that there are only minor differences between the graphs. The normal stress $\tau_{33}$ is not considered because it is almost equivalent to $\tau_{11}$. The graphs show that the normal stresses remain practically unchanged at the end of the cycle, so the error in them can be neglected.

![Figure 2. Normal stress.](image)

Differences are observed in the shear stress graph $\tau_{12}$ in Fig. 3, where residual stresses are present at the end of one cycle of loading.

![Figure 3. Shear stress.](image)
Further estimates are made only for the shear stress. It is clear that with each subsequent cycle, the residual voltage will be increasingly removed from zero at the end of the cycle.

As mentioned in the introduction, to describe the wave pattern of deformation of shock loading of solid bodies, it is sufficient to pass to two or three compression and stretching waves. For the selected cyclic deformation, it suffices to look at how the shear stress graph looks after 3 cycles on Fig. 4.

![Figure 4. Shear stress after 3 cycles.](image_url)

The regularity of the sign of the residual stresses calculated with the help of the Jaumann and Green-Naghdi corotational derivatives is observed: Fig. 3 and Fig. 4.

### 4. Estimates of residual stresses

Further, we estimate the residual stresses after 3 loading cycles of 2024 as an isotropic material (column 2) with further consideration of the anisotropy and estimation of the differences in formulas (7) and (9): $\Delta \bar{P}$ is the contribution of additional terms for the corotational derivatives in the case of anisotropy of the material (column 3).

If we carry out loading in the direction of weak elastic properties, then the residual stresses, taking into account the anisotropy, will increase modulo.

| Derivative                | Isotropic case | Anisotropic case |
|---------------------------|----------------|------------------|
| Jaumann $\Delta f \sigma_{12}$ | $\langle \Delta f \sigma_{12} \rangle_{\text{iso}}$ = 2.025 MPa | $\langle \Delta f \sigma_{12} \rangle_{\text{iso}} + \Delta \bar{P}$ |
| Green-Naghdi $\Delta g \sigma_{12}$ | $\langle \Delta g \sigma_{12} \rangle_{\text{iso}}$ = −1.35 MPa | $\langle \Delta g \sigma_{12} \rangle_{\text{iso}} - \Delta \bar{P}$ |

If we carry out loading in the direction of strong elastic properties, then the residual stresses, taking into account the anisotropy, will decrease modulo.

| Derivative                | Isotropic case | Anisotropic case |
|---------------------------|----------------|------------------|
| Jaumann $\Delta f \sigma_{12}$ | $\langle \Delta f \sigma_{12} \rangle_{\text{iso}}$ = 2.025 MPa | $\langle \Delta f \sigma_{12} \rangle_{\text{iso}} - \Delta \bar{P}$ |
| Green-Naghdi $\Delta g \sigma_{12}$ | $\langle \Delta g \sigma_{12} \rangle_{\text{iso}}$ = −1.35 MPa | $\langle \Delta g \sigma_{12} \rangle_{\text{iso}} + \Delta \bar{P}$ |
The regularity of the sign of the residual stresses is preserved, however, the accounting of the anisotropy affects to the result depending on the choice of the direction of the load. This is demonstrated in Tables 3 and 4.

5. Conclusions

1. For materials with an isotropic symmetry of properties, the magnitude of the residual stress for the Jaumann derivative assumes only positive values, and for the Green-Naghdi derivative - negative values.

2. In the case of strong elastic properties, the contribution of the additional terms taking anisotropy into account reduces the residual stress arising after each loading cycle, and in the case of weak elastic properties - increases.

3. Since residual stresses at the end of the loading cycle have opposite signs for the Jaumann and Green-Naghdi derivatives, then using their linear combination one can reduce the residual stresses to zero.

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