

A Model for Stress Analysis of Elastomer Samples' Crystallisation in a Solid Mechanics Problem Accounting for Superimposed Finite Strains

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Abstract

A mathematical model, method and an algorithm for numerical analysis of stress and strain in elastomeric samples under crystallisation are presented. The stress and strain analysis is performed by means of a CAE Fidesys program module based on the proposed algorithm. The results show that accounting for crystallisation effects is essential for the correct estimation of the stress and strain state of elastomeric samples.

Keywords: Elastomer, incompressible material, finite deformations, crystallisation, superposition, CAE Fidesys

1 Introduction

The problem of analysing the crystallisation of elastomers is important for estimating elastomeric samples' term health, especially for those that are used at low temperatures. There are many types of tyres nowadays, often used in winter when the temperature is about -20 – 30°C . Crystallisation occurs fast enough at that temperature when the elastomeric material is heavily loaded. At present, existing mathematical models do not allow for calculation of the crystallisation effect for elastomeric materials to an accuracy suitable for industrial use. The crystallisation effect is usually determined experimentally, by testing multiple samples. Nevertheless, the efficient development of the tyre industry is impossible without complicated numerical modelling that requires significant computer power. In solid body mechanics, elastomers are considered as incompressible or weakly compressible materials. The computations for those materials are more expensive than for compressible materials [19, 20]. Crystallised elastomers can be considered as composite materials [3].

2 Problem Statement

We solve boundary value problems of nonlinear elasticity for a volume V_0 in its initial state (before deformation).

The equilibrium equation and boundary conditions could be represented in the initial state coordinates.

The equilibrium equation in coordinates of the initial state:

$$\overset{0}{\nabla} \cdot \mathbf{P} + \rho_0 \mathbf{f} = 0 \quad (1)$$

Here $\mathbf{P} = (\det \mathbf{F}) \boldsymbol{\sigma} \cdot \mathbf{F}^{-T}$ is the first Piola-Kirchhoff stress tensor; \mathbf{f} is the vector of body force; ρ_0 is the density in the initial (undeformed) state, $\overset{0}{\nabla}$ is the gradient operator in the initial state, dot denotes the tensor contraction. Superscript T is the sign of transposition, and the superscript $-T$ denotes the superposition of inverse and transposition.

The boundary conditions in coordinates of the initial state (when there is a pressure P applied at the boundaries) could be represented as:

$$\mathbf{v} \cdot \mathbf{P} \Big|_{\gamma} = -PJ\mathbf{v} \cdot \mathbf{F}^{-T} \quad (2)$$

where γ is the boundary at the initial state that becomes Γ in the current state, and \mathbf{v} is normal to γ ; $\boldsymbol{\sigma}$ is the true total stress tensor (Cauchy stress tensor); $J = \det \mathbf{F}$

is the volume ratio ($J = 1$ for incompressible materials); \mathbf{F} is the deformation gradient.

The mechanical properties of incompressible, isotropic, nonlinear-elastic material are described by the Mooney-Rivlin constitutive relations:

$$\boldsymbol{\sigma} = 2C_1\mathbf{B} - 2C_2\mathbf{B}^{-1} - p\mathbf{E} \quad (3)$$

where C_1 and C_2 are empirically determined material constants; $\mathbf{B} = \mathbf{F} \cdot \mathbf{F}^T$ is the Finger deformation tensor; p is a Lagrange multiplier that is independent on strains; \mathbf{E} is the second-order identity tensor. The superscript T denotes the transposition.

3 Elastomer crystallisation modelling

Rubber and other polymers' deformations are followed by their partial crystallisation. Crystallisation of elastomers is a phase transition of the first kind in which the density of the material varies and its elastic properties significantly change: the rigidity of the crystalline phase is 2–3 orders of magnitude greater than the rigidity of the amorphous phase [1, 2, 5, 6, 16]. At the macroscopic level the crystallisation process is described by the Avrami equation [5, 16], the parameters of which depend strongly on the pre-strain and temperature. One of the models of elastomer crystallisation describes crystallisation as an evolutionary process, proposed in [13]. Apparently, for a description of strain-induced elastomer crystallisation, one can use a model similar to the models proposed in [10-12]. It should be noted that such models are quite complicated for numerical implementation for bodies with stress concentrators, especially for bodies made of incompressible and slightly compressible materials, which include elastomers.

In this paper we propose a simplified approach to modelling the crystallisation of elastomers, based on the theory of multiple superposition of large deformations [7-9]. The following is a brief description of the theory. Let us distinguish N states of a body: initial (undeformed) state; $(N-2)$ intermediate states, for which body goes step-by-step by successively applied external effects or due to internal processes taking place in it; the final or current state, to which body goes after the application of all external loads to it in the predetermined order and after the completion of all internal processes. The states are numbered from 0 to N . The transition of the body from state m to the state n is characterised by the deformation gradient $\mathbf{F}_{m,n}$. If the body transition from the initial to the current state is considered, then it is said about the full deformation gradient; if the body transition from the intermediate state to another intermediate state or to the current state is considered, then it is said about the additional deformation gradient.

The proposed model of elastomer crystallisation in the theory of superposition of large deformations can be formulated as follows. At the initial (undeformed) state, there is no stress and strain in the body. Further, under the influence of external loads, the initial deformations occur in the body, and the body

passes to the first intermediate state. At this state, using a criterion, the part of the body is determined in which crystallisation occurs (for example, it may be a region in which maximum principal extension exceeds some critical value). The body material properties change in this region. The constitutive relations change too (or some constants of the material change). In addition, constitutive relations in this region include additional strains but not full strains.

It is known [1, 2] that the elastic modulus of elastomeric materials at crystallisation increases by 2 orders. That's why in this article we suppose that the properties of elastomer in crystallisation region are described by constitutive equations of the same type as the material properties of non-crystallised elastomer but with elastic modulus increased in 50 times.

Due to the changing of the material properties in the region where crystallisation occurs, additional deformations appear that are superimposed on the initial deformations. The body then passes to the next (second) intermediate state.

The empirically determined relations between temperature, crystallisation time, and the stress at which crystallisation occurs are given in [1, 2]. Specifying temperature and crystallisation time, we can determine the value of stress at which crystallisation occurs. This value of stress is used as a criterion of crystallisation. The regions in which maximal principal stress exceeds this value are assumed to be regions of crystallisation.

The process of loading can be extended. New external loads can be applied to the body, which leads to the appearance of the new additional strains that are superimposed on the existing ones. The body then passes to the next (third) intermediate state. The new crystallisation regions are determined in this state. The material properties change in this region, leading to additional deformations of the body. The body then passes to the next (fourth) intermediate state. Then, additional loading of the body followed by the formation of new crystallisation regions could be repeated multiple times.

The proposed model is a significant simplification of the real processes occurring during crystallisation of elastomers. However, this model allows one to consider the most important phenomena (in terms of solid mechanics) that occur during crystallisation of elastomers. The first is a multiple increase in stiffness modulus under the transition of the material to the crystalline state. Another is the relaxation (decrease) of stresses that occurs during crystallisation.

If, after crystallisation, stress depends on the total strains, then with the elastic modulus increase, stress will be increased as many times as the modulus is increased. Then, the elastic energy stored in material would be increased many times too. However, such phenomena are not observed in experiments. The stress is reduced during crystallisation [5, 16] and the energy is released and converted into heat. Therefore, it seems reasonable to assume that after crystallisation the stresses may depend on the additional strains that have occurred after the material passes into the crystalline state. In other words, using the terminology of phase transformation theory, it is assumed that the transformation strains coincide with the initial strains that take place in elastomers before crystallisation.

In the calculations below, it is assumed that the mechanical behaviour of elastomers before crystallisation is described by the constitutive equations (3) for incompressible material. The mechanical behaviour of elastomers after crystallisation is described by the same constitutive equations, but the generalised Finger deformation tensor $\mathbf{B}_{m,n} = \mathbf{F}_{m,n} \cdot \mathbf{F}_{m,n}^T$ is used in these equations as a measure of strains (m is the number of state in which crystallisation occurs, and n is the number of current state). In this paper we used the constitutive equations for the Mooney-Rivlin solid in order to describe the mechanical properties of the crystallised elastomer, but the values of elastic constants are substantially greater than for the non-crystallised state.

The problem statement for the n -th state in coordinate basis of the k -th state consists of the following equations:

The equilibrium equation

$$\nabla \cdot [J_{0,n}^{-1} \mathbf{F}_{k,n} \cdot \mathbf{S}_{0,n}] = 0 \quad (4)$$

Boundary conditions

$$\mathbf{v} \cdot \mathbf{S}_n \Big|_{\Gamma_k} = -PJ_{0,n} \mathbf{v} \cdot \mathbf{F}_{k,n}^{-1} \cdot \mathbf{F}_{k,n}^{-T} \quad (5)$$

$$\mathbf{S}_{0,n} = J_{0,n} [\mathbf{F}_{k,n}]^{-1} \cdot \boldsymbol{\sigma}_{0,n} \cdot [\mathbf{F}_{k,n}]^{-T} \quad (6)$$

Constitutive equations (3) are used for a region without crystallisation:

$$\boldsymbol{\sigma}_{0,n} = 2C_1 \mathbf{B}_{0,n} - 2C_2 \mathbf{B}_{0,n}^{-1} - p_{0,n} \mathbf{E} \quad (7)$$

But for a crystallisation region the constitutive equations are written as

$$\boldsymbol{\sigma}_{0,n} = 2C_1 \mathbf{B}_{m,n} - 2C_2 \mathbf{B}_{m,n}^{-1} - p_{0,n} \mathbf{E} \quad (8)$$

Geometrical relations

$$J_{0,k} = \det \mathbf{F}_{0,k} \quad (9)$$

$$\mathbf{F}_{0,n} = \mathbf{F}_{k,n} \cdot \mathbf{F}_{0,k} = \mathbf{F}_{m,n} \cdot \mathbf{F}_{0,m} \quad , \quad \mathbf{F}_{k,k+1} = \mathbf{I} + \nabla \mathbf{u}_{k+1} \quad (10)$$

$$\mathbf{B}_{0,n} = \mathbf{F}_{0,n} \cdot \mathbf{F}_{0,n}^T \quad (11)$$

$$\mathbf{B}_{m,n} = \mathbf{F}_{m,n} \cdot \mathbf{F}_{m,n}^T \quad (12)$$

Here m is the number of state in which crystallization occurs; $\mathbf{F}_{k,n}$ is the deformation gradient in transition from the k -th state to the n -th state; $\mathbf{u}_{k+1} = \mathbf{r}^{k+1} - \mathbf{r}^k$ is the displacement vector defining the transition from the k -th state to the n -th state; \mathbf{r}^n is the radius-vector of a particle in the n -th state; $J_{0,k}$ is the relative volume variation in transition from the initial state to the k -th state; $\boldsymbol{\sigma}_{0,n}$ is the true stress tensor for the n -th state; (at $n=1$, this tensor is the Cauchy stress tensor); $\mathbf{S}_{0,n}^k$ is the generalised stress tensor in the base of the k -th state under transition from the initial state to the n -th state; at $k=0$, this tensor is the second Piola-Kirchhoff stress tensor; $\mathbf{B}_{k,n}$ is the generalised Finger deformation tensor that describes strains accumulated in transition from the k -th state to the n -th state; \mathbf{v}^k is the normal vector to the boundary Γ_k of a body in the k -th state; $\lambda_{0,n}$ is a Lagrange multiplier in transition from the initial state to the k -th state.

4 Numerical solution and results

The finite-element method (FEM) is used to solve the given equation system. The Newton method is used for linearisation. At each step of this method we solve a linear algebraic equation system (LAES) with unknown vectors \mathbf{U} and \mathbf{P} (where \mathbf{U} is the vector of nodal displacements and \mathbf{P} is the vector of nodal pressures). That system could be solved by the Uzawa method [14, 17].

The proposed algorithm was implemented as a program module (plug-in) in CAE Fidesys [4, 18].

As a model numerical example, the problem of the plane strain of the body with an elliptic hole is considered. The size of the plate is l by l , and the lengths of the semi-axes of the ellipse are equal to $0.1l$ and $0.025l$. The shape of the body, the finite-element mesh, and the scheme of loading are shown in Figure 1. The minor and major axes of the ellipse coincide with the x and y axes, respectively. The tensile load $\sigma_{yy} = 0.05$ MPa is applied to the horizontal sides of the plate, and two other sides are fastened so that the displacement of these sides along the x -axis is equal to zero. The material constants before crystallization are $C_1 = 0.9$ MPa, $C_2 = 0$. The material constants after crystallization are $C_1 = 50$ MPa, $C_2 = 0$.

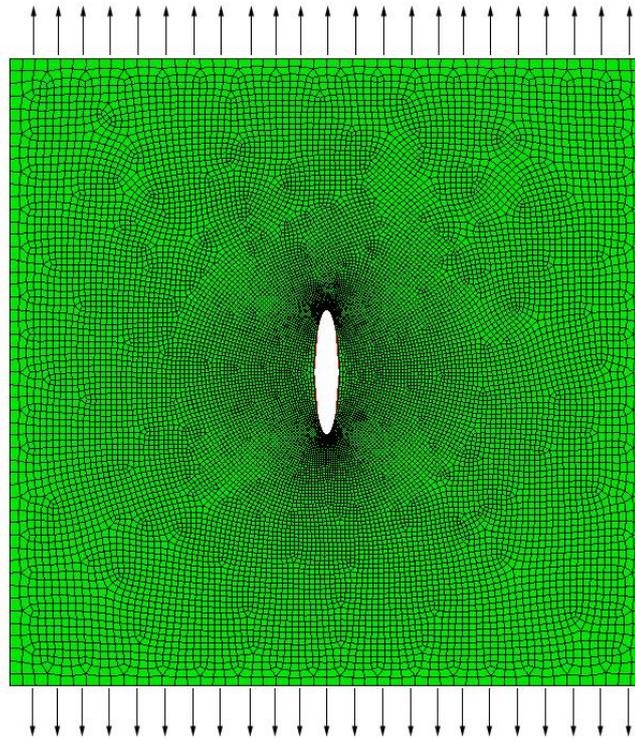


Fig. 1. The computational model and the finite-element mesh

The computations show that the maximal principal stress in the body before crystallisation is equal to 0.46 MPa. This value is multiplied by a factor 0.95, and the obtained value is considered as a criterion of crystallisation. A region in which the maximal principal stress exceeds this value is determined. This region is highlighted in Figure 2 (only the part of the body near the tip of the ellipse is shown in this Figure). The shape of this region fits qualitatively with experimental results [15]. The stress analysis for the body with the crystallised region is performed. The material properties in the crystallised region are described by the constitutive equation (8).

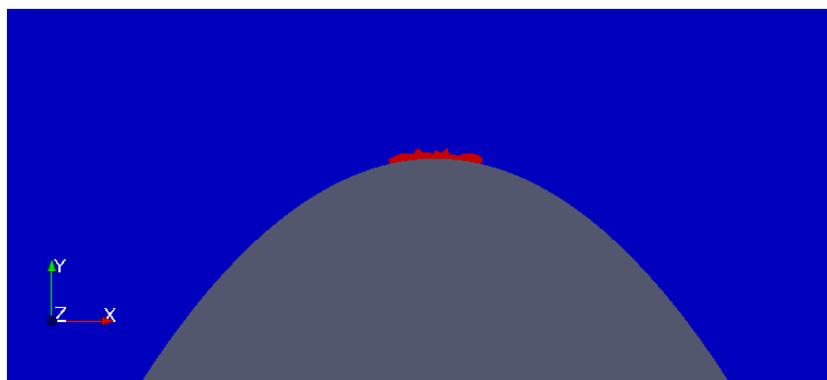


Fig. 2. The region in which crystallisation occurs.

Some results of stress analysis after crystallisation are shown in Figures 3-6. The distribution of principal stresses and strains near the tip of the elliptic hole are shown in these Figures. The stresses are given in MPa.

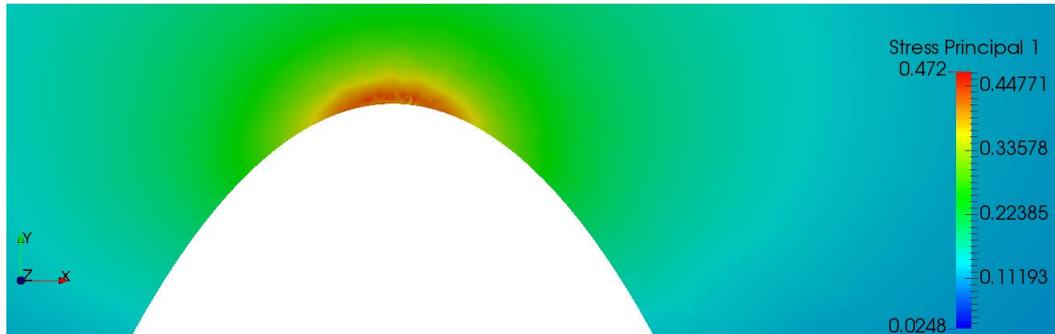


Fig. 3. The distribution of the first principal stress near the tip of the hole

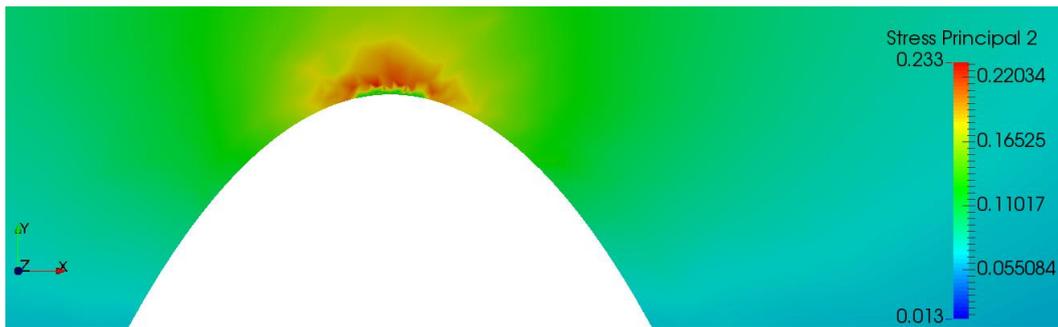


Fig. 4. The distribution of the second principal stress near the tip of the hole

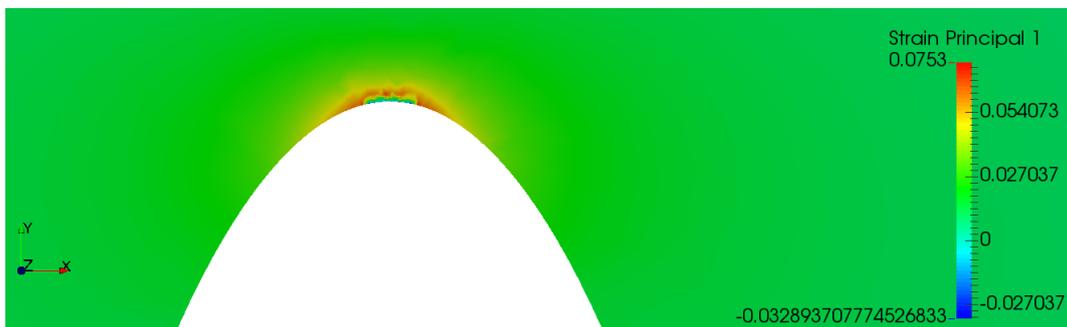


Fig. 5. The distribution of the first principal strain near the tip of the hole

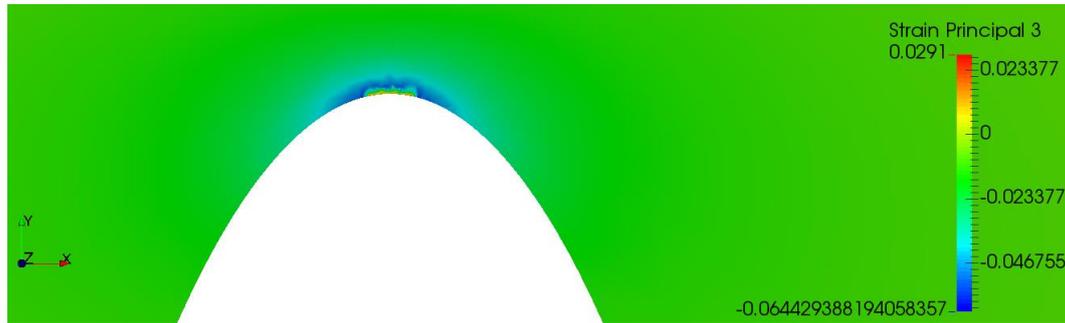


Fig. 6. The distribution of the third principal strain near the tip of the hole

Note that the second principal strain is equal to zero due to plane strain condition.

The obtained results show the workability of the proposed model.

5 Conclusions

A mathematical model that describes the stress and strain state of elastomeric samples under stress-induced crystallisation has been developed. This model is based on the theory of repeated superposition of finite strains. A computational procedure has been proposed that allows numerical estimation of stress and strain state of elastomeric samples under finite strains accounting for crystallisation and superposition effects. Amorphous elastomer is considered as an incompressible material. The proposed model has been implemented in CAE Fidesys. Accounting for nonlinear and crystallisation effects is essential for the correct stress and strain analysis of elastomeric samples undergoing large strains and experiencing the effect of crystallisation.

Acknowledgements. This work was financially supported by the Ministry of Education and Science of the Russian Federation in the framework of the agreement No. 14.579.21.0007 for a grant (unique identifier of the project RFMEFI57914X0007). Investigations were carried out within the Fidesys company — a grantee of the Ministry of Education and Science of the Russian Federation.

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Received: August 4, 2016; Published: September 17, 2016