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DEFORMATION DYNAMICS OF THE SOLID STRUCTURAL UNIT FROM AN EXTERNAL ACTION

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In this work we present the model for study the solid deformation dynamics based on the structural unit method. The solution results of some model equations are given. Time dependence of the sections relative displacement of a structural unit during the uniaxial longitudinal deformation is graphically represented.

Keywords: *SOLID DEFORMATION, STRUCTURAL UNIT METHOD, UNIAXIAL LONGITUDINAL DEFORMATION, MATHEMATICAL PROCESSES SIMULATION, GENERALIZED POTENTIAL.*

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1. INTRODUCTION

The present-day world is in significant want of new structural materials, and the requirements to their strength, operating life, high-temperature strength, stability against dynamic loads and to other characteristics rise. Under these circumstances the development of theoretical justification, practical methods of research, analysis and synthesis, and the methods of modern materials production as well is the task of fundamental and applied science. Computational techniques have been essentially developed, what, in its turn, gave an application possibility of new methods and models for theoretical study of properties of the solids. The study of kinetic aspects of deformation process, sample loading-rate effect on the coefficients of its equation of state, and different short-term processes are especially relevant. The experimental investigations are also carrying out in this field now [1-3], which can be used for experimentally-theoretic models, and for study the mathematical models with respect to their adequacy of reality as well.

2. STATEMENT OF THE PROBLEM

The existing methods of mathematical simulation of the processes in continuums suppose using the continual partial differential equations, solving which the difference schemes [4-6] are used. During such approach it is difficult to experimentally keep track the changes of partial derivatives data from the system basic parameters and find the physics of phenomena in process of matter transition from one state to another. One of new methods in the study of deformation dynamics is the particle method, proposed in [7], which is based on using of the ordinary differential equations, with the help of which the dynamics of particles motion subject to their interaction is described. With appearance of modern multi-processor computation systems this method had been developed, but its fundamental defect is non-

applicability to the real crystal structures of the metals, conditioned by considerable complexity of transition from the plane problem to the solution of equation for three-dimensional structure.

The aim of the present work is development of the method, which allows to study the solid deformation dynamics on the base of theoretical model and experimental data.

3. STRUCTURAL UNIT METHOD

Proposed in the present work the structural unit method (cell method) is similar to the particle method, but differs by the following: the structural unit consists of individual particles, which configuration depends on matter structure and essentially influences on its properties. Configuration can be obtained using the diffraction method [8, 9]. In this work we consider the uniaxial deformation dynamics of the face-centered cubic (fcc) structure of metals and alloys, but this method is applicable to other types of crystal structures [10-12] as well. As the interaction potential between the structural unit elements (atoms) the generalized potential of the type of $\Pi(r) = -D(e^{-2Ar} - 2e^{-Ar})$ is used, which is adapted to the real experimental investigations. The potential parameters essentially depend on thermodynamic parameters and are connected with the macroscopic properties of investigated solid: $D(P, T)$ is the dissociation energy (the bond breaking energy); r is the vector of atom displacement from equilibrium position; A is the constant, dependent on the nature of corresponding matter. We have to note, that it is possible to use other potentials, particularly: the Lennard-Jones potential, the Morse potential, the spline potential, the generalized one, and others, which are adapted to the defined matter structure [13-14].

Consider the fcc metal lattice, where the external stretching force F is applied to its face. Under acting of this force the structural unit (fcc cell) is deformed in force direction, and in this case the interatomic distances gradually change, since the interacting forces $f(r) = -d\Pi(r)/dr$ between the lattice atoms start acting, conditioned by the interaction potential $\Pi(r)$, where r is the vector of interatomic distance changes.

The resultant interaction force, acting on the i-th atom in a cell, is the vector sum of all forces, acting on the atom in deformation direction.

$$\vec{f}_{Pi}(\vec{r}_{ik}) = \sum_{i=1, i\neq k}^{n} \vec{f}_{Pi}\,(r_{ik}) \cos(\hat{r_{ik}, \vec{F}}), \qquad (1)$$

where $\cos(\hat{\vec{r}_{ik}, \vec{F}})$ is the cosine of angle between the vector $\vec{r}_{ik}$ and the motive force vector $\vec{F}$, $\vec{r}_{ik}$ is the distance between the i-th and the k-th atoms in the corresponding cell face ($i \neq k$), n is the number of atoms in a cell, $\vec{f}_i(\vec{r}_{ik})$ is the interaction force vector of the i-th cell atom with the other atoms in a cell. During the deformation atoms in sections will displace from the equilibrium position that will lead to the changes of interatomic distances and interaction forces $\vec{f}_i(\vec{r}_{ik})$. Radiuses $\vec{r}_{ik}$ are interconnected with the longitudinal $\delta_{||}$ and the lateral $\delta_{\perp}$ cell deformations, which can be determined experimentally if consider the forces, acting in the cell sections (see Fig. 1).

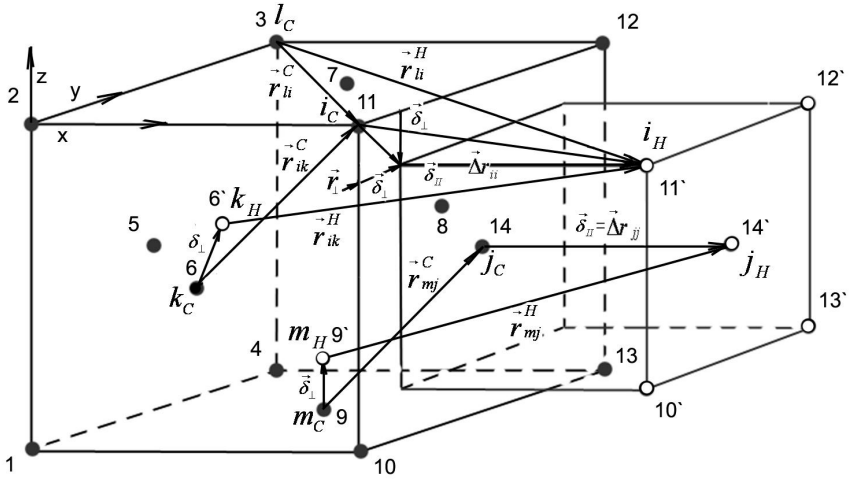

Fig. 1 *– Diagram of the forces, acting in the sections of deformed cell*

In vector form the interconnection of coordinate vectors $\vec{r}_{ik}$ and $\vec{r}_{mj}$ with displacement vectors $\vec{\delta}_{||}$, $\vec{\delta}_{\perp}$, $\Delta\vec{r}_{ii}$, $\Delta\vec{r}_{jj}$ for the interaction of i-th and k-th, m-th and j-th, l-th and i-th atoms, entered into the structural unit, will be written in the form:

$$\begin{aligned}
\vec{r}^{\,C}_{ik} + \Delta\vec{r}_{ii} + \vec{\delta}_{||} &= \vec{r}^{\,H}_{ik} + \vec{\delta}_{\perp}, \\
\vec{r}^{\,C}_{li} + \vec{r}_{\perp} + \vec{\delta}_{||} &= \vec{r}^{\,H}_{li}, \\
\vec{r}^{\,C}_{mj} + \Delta\vec{r}_{jj} &= \vec{r}^{\,H}_{mj} + \vec{\delta}_{\perp}, \\
\Delta\vec{r}_{ii} &= \Delta\vec{r}_{jj} + \vec{r}_{\perp}, \\
\Delta\vec{r}_{jj} = \vec{\delta}_{||} &= \Delta\vec{r}_{ii}, \\
\vec{r}_{\perp} &= \vec{\delta}_{\perp}\sqrt{2},
\end{aligned} \tag{2}$$

where $\vec{r}^{\,C}_{ik}, \vec{r}^{\,C}_{mj}$ are the radius-vectors between the corresponding atoms of a cell before deformation (old), $\vec{r}^{\,H}_{ik}, \vec{r}^{\,H}_{mj}$ are the radius-vectors between the corresponding atoms of a cell after deformation during the given time interval (new).

In Fig. 1 we represent the interconnection of vectors, which condition an interaction between the corresponding atoms, entered into the structural unit before and after interaction of the i-th, k-th, m-th, j-th, l-th atoms (atoms are assigned the numbers 1...14, the stroke denotes position after deformation), with vectors of the longitudinal δ_{II} and the lateral $\delta_{\perp}$ cell deformations, where i_C, k_C, m_C, j_C, l are the notations of the particles (atoms) in initial state, and i_H, k_H, m_H, j_H, l_C are the notations of the corresponding atoms in a new state, $\vec{r}^{\,C}_{ik}, \vec{r}^{\,C}_{mj}, \vec{r}^{\,C}_{li}, \vec{r}^{\,H}_{ik}, \vec{r}^{\,H}_{mj}, \vec{r}^{\,H}_{li}$ are the radius-vectors between the corresponding atoms in an old and a new (occurred due to deformation during the given time interval) states; $\Delta\vec{r}_{ii}, \Delta\vec{r}_{jj}$ are the resultant vectors of the corresponding atoms deformation.

Substituting $\vec{r}_{ik}^{H}$ and $\cos(\hat{\vec{r}_{ik}, \vec{F}})$ into expression (1) for the force $\vec{f}_i(\vec{r}_{ik})$ and summarizing over the directions x, y, z for all cell atoms we obtain

$$\begin{aligned}
&\text{stretching forces } \vec{f}_{xi} = \sum_{i=1, i\neq k}^{n} \vec{f}_i(\vec{r}_{ik}) \cos(\hat{\vec{r}_{ik}, \vec{x}}) \text{ – along the } x \text{ axis;} \\
&\text{pressing forces } \vec{f}_{yi} = \sum_{i=1, i\neq k}^{n} \vec{f}_i(\vec{r}_{ik}) \cos(\hat{\vec{r}_{ik}, \vec{y}}) \text{ – along the } y \text{ axis;} \qquad (3) \\
&\qquad\qquad \vec{f}_{zi} = \sum_{i=1, i\neq k}^{n} \vec{f}_i(\vec{r}_{ik}) \cos(\hat{\vec{r}_{ik}, \vec{z}}) \text{ – along the } z \text{ axis.}
\end{aligned}$$

Under consideration of uniaxial longitudinal deformation the fcc cell can be conditionally divided into two faces and one section, respectively, the face 1, the face 3 and the section 2 (see Fig. 2). Proceeding from the symmetry, the resultant force, acting on the faces and the section along the deformation vector, subject to (1) will be written as:

$$\begin{aligned}
&\text{for the face 1} \qquad \vec{f}_{x1} = \frac{1}{4}\sum_{i=1}^{4} \vec{f}_{xiP} + \vec{f}_{x5P}; \\
&\text{for the section 2} \qquad \vec{f}_{x2} = \frac{1}{2}\sum_{i=6}^{9} \vec{f}_{xiP}; \qquad (4) \\
&\text{for the face 3} \qquad \vec{f}_{x3} = \frac{1}{4}\sum_{i=10}^{13} \vec{f}_{xiP} + \vec{f}_{x14P}.
\end{aligned}$$

Forces, acting in transverse direction of deforming force F, in the cell planes 1, 2, 3, expressed in the terms of deformation vectors and coupling stiffness coefficients $k_{\perp 1}$, $k_{\perp 2}$, can be written as follows:

in the faces 1, 3:

$$\begin{aligned}
f_{ik} &= -k_{\perp 1}\sqrt{\delta_y^2 + \delta_z^2} = -k_{\perp 1}\delta_\perp\sqrt{2} \text{ (for } i = 1\text{-}4 \text{ and } i = 11\text{-}14), \\
f_{ik} &= -k_{\perp 2}\delta_y = -k_{\perp 2}\delta_\perp \text{ (for } i = 6\text{-}9), \qquad (5)
\end{aligned}$$

$\delta_\perp = \delta_y = \delta_z$, $k_{\perp 1}$ and $k_{\perp 2}$ are the coupling stiffness coefficients for atoms in the section 2 and the faces 1,3.

The directions of deformation vectors, acting in the cross-sections 1, 2, 3 in a structural unit, are showed in Fig. 2.

It is follows from (5), that stretching forces in the sections 1, 2, 3 are different, and, correspondingly, the stiffness coefficients will be different as well.

For study the deformation dynamics (kinetics) we consider displacement of the cell faces and sections under the external force action. Also we assume that the cell faces and sections move together with atoms, located into them, parallel to each other. This gives an opportunity to use the equivalent calculation model of displacements of the cell faces and sections.

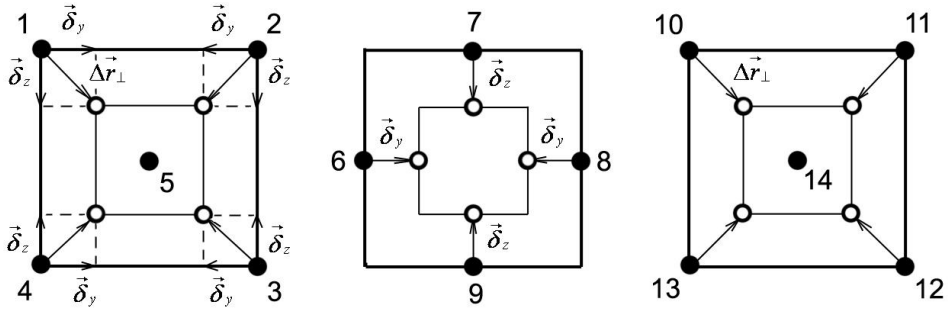

Fig. 2 *– Schematic representation of the deformation vectors directions*

Taking into account that the energy scattering coefficient in a cell β and the stiffness coefficient of interatomic bond k are functions of the deformation vector that is $\beta(r)$ and $k(r)$, the equation of motion of reduced masses will be essentially nonlinear with variable coefficients. In the linearized form the equations of motion of reduced masses in a cell (see Fig. 3), expressed in terms of deformation velocity $d\Delta r/d\tau$ for the i-th time moment with initial conditions $\tau = 0$ and $\Delta\dot{r} = 0$, can be written as follows:

for the mass m_1^*

$$\frac{d\Delta\dot{r}_{1i}}{d\tau} + 2\beta_{1i-1}\Delta\dot{r}_{1i} + \int_0^{\tau} \frac{\Delta k_{1i-1}}{m_1^*}\Delta\dot{r}_{1i}dr = \frac{F(\tau)_i}{m_1^*}; \tag{6}$$

for the mass m_2^*

$$\frac{d\Delta\dot{r}_{2i}}{d\tau} + 2\beta_{i-1}\Delta\dot{r}_{2i} + \int_0^{\tau} \frac{\Delta k_{2i-1}}{m_2^*}\Delta\dot{r}_{2i}dr = \frac{F(\tau)_i}{m_2^*}, \tag{7}$$

where $\Delta\dot{r}_i = d\Delta r_i/d\tau$ is the deformation velocity in the i-th time moment for the corresponding masses; β_{1i} and β_{2i} are the scattering (dissipation) coefficients under the corresponding deformation Δr_i; Δk_{1i} and Δk_{2i} are the stiffness coefficients of interatomic bond under the corresponding deformation Δr_i; $F(\tau)$ is the time-varying external force; f_{12} and f_{23} are the interatomic interaction forces, acting in the sections 1, 2, 3 along the deformation force.

Forces f_{12} and f_{23} are calculated using expressions (1) and (4) for every time moment. An increment of deformation vector in the i-th time moment for the corresponding masses can be evaluated with expression

$$\Delta r_i = \int_0^{\tau} \Delta r\, dr\,. \tag{8}$$

The correlation of interatomic distances r_{12}, r_{23}, r_{34} in the i-th time moment during the reduced masses displacement from the equilibrium position can be presented as follows:

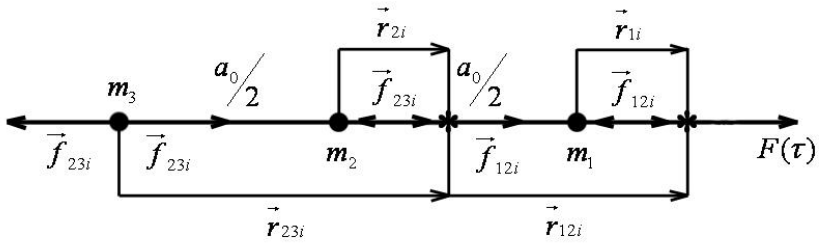

Fig. 3 *– Forces action on the reduced masses in an arbitrary time moment under the external force* $\vec{F}(\tau)$ *influence. Dots denote the initial positions of reduced masses in a cell; asterisks present the positions of reduced masses in a cell in an arbitrary time moment*

$$r_{12i} = \frac{a_0}{2} + (\Delta r_{1i} - \Delta r_{2i}),\ r_{23i} = \frac{a_0}{2} + (\Delta r_{2i} - \Delta r_{3i})\,. \tag{9}$$

The deformation work of a structural unit (cell) can be expressed with the interaction potentials in a new $\Pi(r_{ik}^H)$ and an old $\Pi(r_{ik}^C)$ states, and with the deformation vectors $\vec{r}_\perp = \vec{\delta}_\perp\sqrt{2}$, $\Delta\vec{r}_{jj} = \vec{\delta}_{||} = \Delta\vec{r}_{ii}$ using expressions (2) as well

$$\begin{aligned} A_{def}^T = \Pi(\vec{r}_{ik}^H) - \Pi(\vec{r}_{ik}^C) = \Delta\vec{r}_{II}\left[\sum_{i=1,i\neq k}^{n}\vec{f}_i(\vec{r}_{ik}^H)\cos(\hat{\vec{r}_{ik}^H},\vec{x}) - \sum_{i=1,i\neq k}^{n}\vec{f}_i(\vec{r}_{ik}^C)\cos(\hat{\vec{r}_{ik}^C},\vec{x})\right] + \\ +\Delta\vec{r}_\perp\left[\sum_{i=1,i\neq k}^{n}\vec{f}_i(\vec{r}_{ik}^H)\cos(\hat{\vec{r}_{ik}^H},\vec{y}) - \sum_{i=1,i\neq k}^{n}\vec{f}_i(\vec{r}_{ik}^C)\cos(\hat{\vec{r}_{ik}^C},\vec{y})\right]. \end{aligned} \tag{10}$$

On the other hand, the deformation work can be calculated using the experimental data

$$A_{def}^E = \Delta\sigma\Delta V_c = \Delta\sigma(V_c^H - V_c^C)\,, \tag{11}$$

where $\Delta\sigma = \Delta F/S(\tau)$ is the stress acting in a cell section, ΔF is the external force applied to a cell face, V_c^H, V_c^C are the cell volumes, respectively, during and before the force ΔF application.

The volumes change can be expressed in terms of the cell size a_0 (at $T = T_0$) and the deformation vectors magnitudes

$$\Delta V_c = 2a_0^2(\Delta r_{||} - \frac{2}{\sqrt{2}}\Delta r_\perp) + 4a_0(\frac{\Delta r_\perp^2}{2} - \frac{2}{\sqrt{2}}\Delta r_\perp\Delta r_{||}) + 4\Delta r_\perp^2\Delta r_{||}\,. \tag{12}$$

It is necessary to experimentally measure the rate of the sample section change with time $dS(\tau)/d\tau = \dot{S}(\tau)$, the sample deformation velocity along the force ΔF direction $dl/d\tau = \dot{l}(\tau)$, the time dependence of the stress, appearing in a sample section $dF(\tau)/dS(\tau) = \sigma(\tau)$ or the same dependences but as functions of deformation vectors.

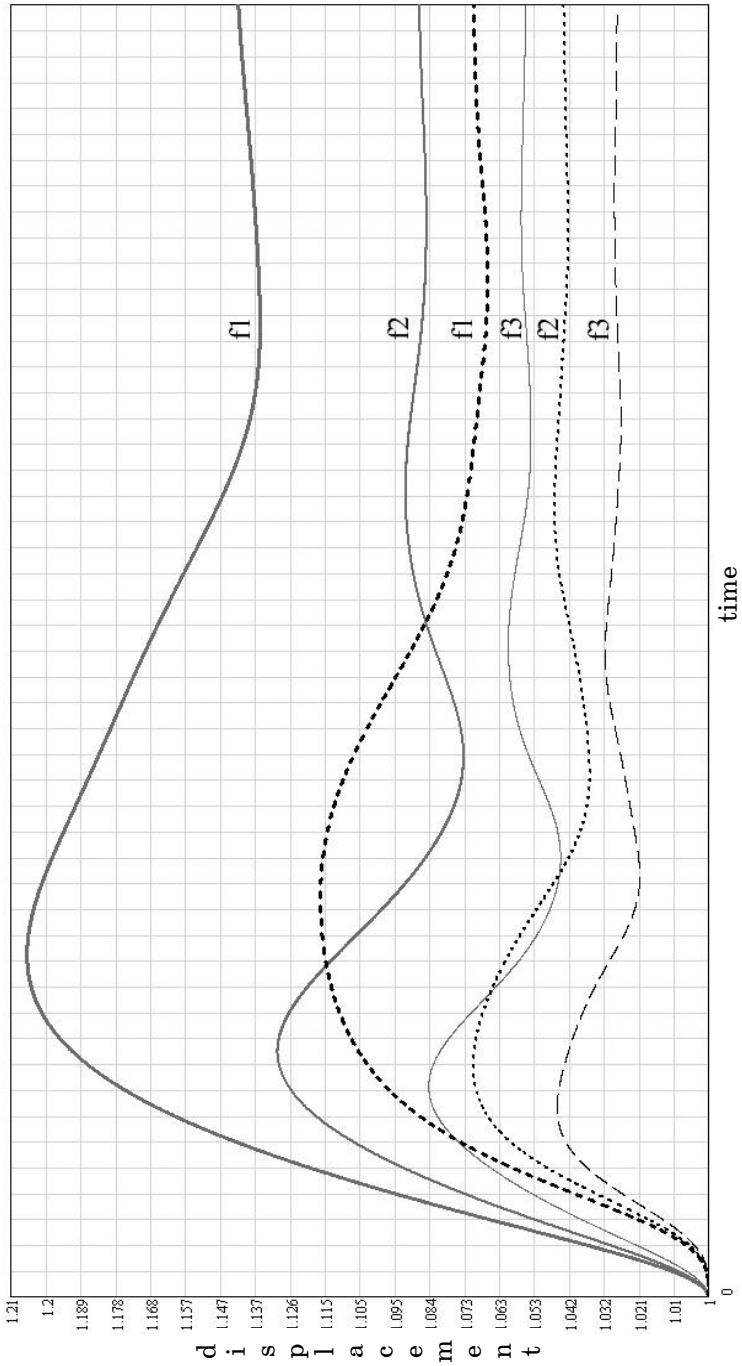

***Fig 4** – Time dependence of the relative displacement of section 2 (dashed line) and face 3 (solid line) of bcc cell during the uniaxial longitudinal deformation under action of different external forces f1 > f2 > f3*

Based on this data it is possible to calculate the cell volume changes with time

$$\Delta V_c(\tau) = \int_{S_0}^{S} \dot{S}(\tau) d\tau \int_{l_0}^{l} \dot{l}(\tau) d\tau \,. \qquad (13)$$

Equations (6)-(8) subject to (1), (4), and (9) allow to investigate the deformation dynamics based on the theoretical model and along with experimental data to generate the functionals: the forcing, the high-speed, and the deformative. Based on expressions (3) and (10)-(13) subject to $d\Pi(r)/dr = -f$ the energy and the forcing functionals are formed, which allow to correct the interaction and the force potential in accordance with experimental data.

4. CONCLUSIONS

Based on the force functional the interacting forces between atoms, entered into the unit fcc-cell, are calculated, what gave a possibility to derive the cell sections displacement with time under the external force F action.

The energy functional is used for description of the energy charac-teristics of the solids: the thermal capacity, the entropy, and the cell internal energy.

The high-speed and the deformative functionals allow based on the experimental investigations of the sample deformation (structural unit) to correct the theoretical energy and forcing functionals relative to the deformation velocity.

Minimization of these functionals gives a possibility to calculate a number of values versus the sample loading rate and create the equation of matter state, which the most closely defines the matter state in the different ranges of deformations, deformation velocities, and temperatures.

As the result of equations (6) and (7) solution the dependencies of the relative displacement of the fcc-cell sections with time during the uniaxial longitudinal deformation under the external force action are obtained. As seen from Fig. 4, the stretching force essentially influences the transient process. Delay of the sections displacement takes place due to inertial properties of a matter. The data of equation allows to study the deformation dynamics of a solid at different values of the external deforming force using parameters of the generalized potential (the dissociation energy A) and experimental data (the cell structure, the interatomic distance, and the external force value). Proposed model allows to explain the nature of deformation phases from the physical point of view.

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