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Advanced Statistical Crystal Plasticity Model: Description of Copper Grain Structure Refinement during Equal Channel Angular Pressing

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Abstract: The grain structure of metals changes significantly during severe plastic deformation (SPD), and grain refinement is the main process associated with SPD at low homologous temperatures. Products made of ultrafine-grained materials exhibit improved performance characteristics and are of considerable industrial interest, which generates a need for the creation of comprehensive grain refinement models. This paper considers the integration of the ETMB (Y. Estrin, L.S. Toth, A. Molinari, Y. Brechet) model, which describes the evolution of an average cell size during deformation into the two-level statistical crystal plasticity constitutive model (CM) of FCC polycrystals. The original relations of the ETMB model and some of its modifications known from the literature were analyzed to obtain an accurate, physically admissible description of the grain refinement process. The characteristics of the grain substructure determined with the framework of the advanced ETMB model were taken into account in the CM in a hardening law. By applying the CM with the integrated ETMB model, numerical experiments were performed to simulate the changes in the grain structure of copper during equal channel angular pressing (ECAP) at room temperature. The results obtained are in good agreement with the experimental data. The ideas about further development of the proposed model are outlined.



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1. Introduction

Mathematical modeling is an effective tool that facilitates the development of modern technological processes of thermomechanical treatment of metals and alloys. Constitutive relations (or constitutive models (CMs)) that characterize the behavior of materials play a key role in mathematical modelling. In recent decades, a multilevel approach to the creation of CMs has been intensively developed based on crystal plasticity [1–6]. In contrast to the macrophenomenological approach, this one allows explicit description of structural changes and, accordingly, the physical and mechanical properties of the materials of finished products and implementation of the physical deformation mechanisms at various scale levels. Thus, multilevel CMs are the most in-demand models for solving the problems associated with technological advances in thermomechanical treatment and with synthesizing new functional materials by severe plastic deformation (SPD) techniques [7,8]. Note that in technological processes, the initial material microstructure (crystallite orientation, phase composition, grain size, etc.) plays a decisive role in the manufacturing of parts and significantly affects the properties of the finished product, so it must be taken into account in the models [9,10]. In accordance with an accepted hypothesis about the relationship between the variables (characteristics) of different levels (a means of combining the elements of the underlying scale level into an element of the overlying scale level), crystal plasticity CMs

are divided into three main groups: statistical [11], self-consistent and direct (the latter are based on the solution of a boundary value problem at the level of grain parts) [12] models.

To date, research on multilevel crystal plasticity CMs able to take into account intragranular dislocation slip (IDS), twinning and rotation of crystallite lattices have been significantly developed [1–6]. An important direction in the development of this class of models is to arrange matters so that CMs would describe other significant deformation mechanisms and the processes occurred during deformation.

It is known that the deformation of polycrystalline metals and alloys during SPD causes a significant change in grain structure. At low homologous temperatures, grain refinement takes place, which will be considered in this paper. By grain refinement (fragmentation), we mean the process of separating grains into fragments (grain integrity at the mesolevel is kept unchanged), triggered by the progressive increase in the misorientation of fragments during plastic deformation, implemented due to dislocation–disclination mechanisms [13–15]. The description of polycrystal grain refinement induced by severe plastic deformation is important because grain size significantly affects the effective properties of the material. When grain size decreases, yield stress increases (in accordance with the Hall–Petch relation) [16], and an increase in ultimate strength can be observed [16,17]. Billets of metals and alloys with submicro- and nanocrystalline structures obtained by SPD at elevated temperatures and low strain rates can be deformed in superplasticity mode, which is extensively used in the technological processes of thermomechanical treatment [18–21]. Therefore, the description of grain structure refinement of various metals and alloys subjected to SPD at low homologous temperatures is a relevant problem.

Following the classification provided in [22,23], grain refinement models can be classified into three main types: continuum models based on the macrophenomenological approach [24–27]; physically-based continuum models [28–35]; and multilevel crystal plasticity models. Recent decades have been marked by the appearance of some modifications of statistical [36–41], self-consistent [42–47] and direct crystal plasticity CMs [48–53], designed to take grain refinement into consideration. Separately, let us note that to describe the processes in question at the microlevel, a popular approach is modeling using the method of molecular dynamics [54–57].

It is worth noting that at present, there is no generally accepted approach to solving this problem. A careful choice of a base model and its modifications is needed, one which will take into consideration the implementation of different mechanisms responsible for the internal structure evolution during severe inelastic deformation and the interactions between these mechanisms. In this connection, it is important to look at all possible ways of checking the correctness of a base model. One aspect of validating the base model is assessing its stability with respect to input data and operator perturbations. In [58], the authors proposed a methodology for the comprehensive evaluation of the stability of multilevel CMs with respect to the perturbations of initial conditions and the influence history and the parametric perturbations of operators; the results of the application case [59] show the stability of a base two-level CM of FCC polycrystals. There is no doubt that this technique can and should be used to assess the validity of extended CMs as well. However, the modification of CMs with consideration of the grain refinement process primarily implies analysis of the correctness of the relations of these crystal plasticity CMs from a physical point of view, which is the subject of the present work.

As a base model, we use here a two-level statistical crystal plasticity CM describing the deformation of FCC polycrystals. The model considers intragranular dislocation slip and rotation of crystallite lattices, and it seems to be more resource-efficient compared to self-consistent and direct models [7,60–62], which enables researchers to employ it in studying real technological processes of thermomechanical treatment. Appropriate constitutive relations are given in Section 2.

Our main concern in this paper is with the integration of the well-known ETMB (Y. Estrin, L.S. Toth, A. Molinari, Y. Brechet) model [28,63], predicting average cell size evolution, into the statistical CM, which has raised a number of issues that must be addressed. As

noted in [64], the dislocation cell structure which emerges during plastic deformation can be seen as a precursor to the final grain structure to be formed under intense strains, particularly under Severe Plastic Deformation. In this regard, the ETMB model is a good basis for constructing more detailed fragmentation models that include an explicit description of the formation of cell blocks and their rotations. On the other hand, the ETMB model in its original form or with a slight correction in the form of equations can also be used for SPD modeling [50,65–67]. In the ETMB model, the mentioned processes are predicted effectively using the phenomenological dependences of the model parameters on the accumulated strain, which directly approximate the experimental data.

It is notable that the literature predominantly reflects the achievements of joint application of the ETMB model and the one-dimensional phenomenological CM, which predict the behavior of effective flow stresses [66,68], the ETMB model and the one-dimensional Taylor model, which only estimates flow stress using the Taylor factor [69–73]. Few works are devoted to cases in which the ETMB model is integrated into direct crystal plasticity CMs [50,65,67,74–76]; note that such models are characterized by high resource intensity. In addition, there is a question of rearranging the grain structure and the field of internal variables during refinement. Thus, it would appear reasonable to construct a numerically efficient full-fledged three-dimensional statistical crystal plasticity CM with an embedded ETMB submodel. Although the results obtained in the framework of the ETMB model are in satisfactory agreement with the experimental data (for copper [63,74,76] and for aluminum [65,68]), an accurate fragmentation description requires a physically meaningful detailed description of implemented processes. For this purpose, we propose a combination of known (proposed by other authors) modifications of some ETMB relations. Section 3 contains the relations of the original ETMB model and some of its modifications and outlines prospects for its development for acquiring an explicit detailed description of grain refinement.

Section 4 presents the results of the identification and verification of the FCC polycrystal CM, as well as the achievements of joint application of the ETMB model and the CM when compared to the experimental data on equal channel angular pressing (ECAP) at room temperature. Note that, in this case, recrystallization occurring in a deformed material is neglected [77–80].

2. Two-Level Statistical Constitutive Model for Describing the Inelastic Deformation of the FCC Polycrystal

In the statistical CM, a representative volume (RV) of a polycrystal that consists of homogeneously deformed crystallites (mesolevel elements) is considered at the macrolevel [6,81–83]. The response of the RV is determined in this case by averaging the stresses obtained at the mesolevel (hereinafter, the macrolevel quantities are denoted by capital letters and the mesolevel quantities by lower-case letters; the crystallite index is omitted for brevity):

$$\mathbf{K} = \langle \boldsymbol{\kappa} \rangle \quad (1)$$

where $\mathbf{K}$ is the weighted Kirchhoff stress tensor at the macrolevel; $\boldsymbol{\kappa} = \overset{\circ}{\rho}/\overset{\circ}{\rho}\boldsymbol{\sigma}$ is the weighted Kirchhoff stress tensor at the mesolevel; $\boldsymbol{\sigma}$ is the Cauchy stress tensor at the mesolevel; $\overset{\circ}{\rho}$, $\overset{\circ}{\rho}$ are the crystallite material densities in the initial (unloaded) and current configurations, respectively; and $\langle \cdot \rangle$ denotes the averaging procedure.

The reference configuration is assumed to be an unloaded state, meaning $\boldsymbol{\kappa} = \mathbf{0}$. The main mechanisms governing the deformation of crystallites are explicitly viewed at the mesolevel. The intergranular slip occurred due to the motion of edge dislocations along close-packed planes in the most closely packed directions (slip systems (SSs)) described by the viscoplastic relation.

The system of equations used to describe the inelastic deformation of one crystallite is written as [6]:

$$\kappa^{cor} \equiv \frac{d\kappa}{dt} + \kappa \cdot \omega - \omega \cdot \kappa = \pi : (\mathbf{I} - \omega - \sum_{k=1}^K \dot{\gamma}^{(k)} \mathbf{b}^{(k)} \mathbf{n}^{(k)}), \quad (2a)$$

$$\dot{\gamma}^{(k)} = \dot{\gamma}_0^{(k)} \left(\frac{\tau^{(k)}}{\tau_c^{(k)}} \right)^m H(\tau^{(k)} - \tau_c^{(k)}), \quad k = 1, \dots, K, \quad (2b)$$

$$\tau^{(k)} = \mathbf{b}^{(k)} \mathbf{n}^{(k)} : \kappa, \quad k = 1, \dots, K, \quad (2c)$$

$$\tau_c^{(k)} = F(\tau_{c0}^{(k)}, l, \rho^{(j)}), \quad j, k = 1, \dots, K, \quad (2d)$$

$$\omega = \omega(\mathbf{I}, \dot{\gamma}^{(k)}), \quad (2e)$$

$$\dot{\mathbf{o}} \cdot \mathbf{o}^T = \omega, \quad (2f)$$

$$\mathbf{I} = \hat{\nabla} \mathbf{v}^T = \hat{\nabla} \mathbf{V}^T = \mathbf{L}, \quad (2g)$$

where the upper index *cor* denotes the corotational derivative independent of the choice of a reference frame; π is the elastic property tensor of the crystallite, the components of which are constant in the moving coordinate system, which rotates with a spin ω and specifies (quasi) rigid motion (a corotational derivative) [84]; $\mathbf{I} = \hat{\nabla} \mathbf{v}^T$ is the velocity gradient of the mesolevel; $\mathbf{b}^{(k)}$ and $\mathbf{n}^{(k)}$ are the unit vectors of the slip direction and the normal relative to the slip plane k (in the current configuration) of edge dislocations; K is the doubled number of the crystallographic slip systems; $\dot{\gamma}^{(k)}$ is the shear rate for the slip system k ; $\dot{\gamma}_0^{(k)}$ is the shear rate for the slip system k when the shear stress reaches its critical value; $\tau^{(k)}$, $\tau_c^{(k)}$ are the shear and critical shear stresses for the slip system k ; m is the strain rate sensitivity exponent of the material in the dislocation slip mode; $H(\cdot)$ is the Heaviside function; $F(\cdot)$ is the function for calculating critical shear stresses along the slip systems (a hardening law, described below); $\tau_{c0}^{(k)}$ is the initial critical stress for the slip system k ; l is the average cell size (determined by means of the ETMB model); $\rho^{(j)}$ – is the dislocation density for the slip system j (for all slip systems, this density is equal to $\rho^{(j)} = \frac{\rho}{K/2}$, where the ρ is determined by means of the ETMB model, a detailed description of which is given in Section 3); and $\mathbf{o}$ is the tensor of actual orientation of the moving coordinate system with respect to the fixed laboratory coordinate system (LCS). Note that in [85,86], instead of using the corotational derivative in (2a), the authors explicitly say that they use a linear constitutive relation in a local coordinate system of crystallites.

As a relation (2d), we use in this study a hardening law [87] where the critical stresses are represented by the sum of terms describing the influence of various type obstacles on the dislocation slip:

$$\tau_c^{(k)} = \tau_{c0}^{(k)} + \tau_{cMHP}^{(k)} + \tau_{cBH}^{(k)}, \quad k = \overline{1, K}, \quad (3a)$$

$$\tau_{cMHP}^{(k)} = k_{MHP} / l, \quad k_{MHP} = \alpha_{MHP} K_r G b, \quad (3b)$$

$$\tau_{cBH}^{(k)} = \sum_{i=1}^K \Omega^{(ki)} \alpha_{BH} G b \sqrt{\rho^{(i)}}, \quad (3c)$$

where (3b) is the modified Hall–Petch relation [66,88–95]; α_{MHP} is the constant; K_r is the constant in the original ETMB model, depending on the strain in the advanced model (relation (20)); G is the shear modulus; b is the Burgers vector modulus; (3c) is the relation

similar the so-called Bailey–Hirsch relation [96–98], which describes the interaction between dislocations; $\Omega^{(ki)}$ is the components of the matrix of interaction between dislocations on the slip system k and dislocations in the slip system i (1 for coplanar slip systems, and q_{lat} for non-coplanar slip systems); and α_{BH} is the Bailey–Hirsch parameter. Since dynamic recovery is not significant for materials with low/medium stacking fault energy at room temperature [99,100] (the case considered in this paper), its effect is ignored in the hardening law (3).

In [82], the rotation of crystallite lattices was described in terms of Taylor’s spin model. Thus, we have

$$\boldsymbol{\omega} = \frac{1}{2}(\mathbf{1} - \mathbf{I}^T) - \frac{1}{2} \sum_{k=1}^K \dot{\gamma}^{(k)} (\mathbf{b}^{(k)} \mathbf{n}^{(k)} - \mathbf{n}^{(k)} \mathbf{b}^{(k)}). \quad (4)$$

Note that the approach in which the moving coordinate system is associated with the symmetry elements of the crystal lattice [84,101] seems to be more physically substantiated in describing the lattice rotation. It was shown in [102] that these spin models produce mostly similar results, only differing slightly from those obtained with the model of the rotation determined by orthogonal tensor in the polar decomposition of the elastic component of the deformation gradient [103]. Taylor’s spin model was used because it can easily be implemented.

In this paper, we use the constitutive model formulated in rate form and written in terms of the actual configuration, which yields results close to those obtained by the formulation in terms of the unloaded configuration [103–108]. In [109,110], the authors described in detail these models and, with intent to establish a relationship between them, used the formulation with an explicit separation of the rigid moving coordinate system in the multiplicative representation of the deformation gradient [84,111].

3. Description of the Aspects (Conditions), Original and Modified Relations of the ETMB Model

Grain refinement by severe plastic deformation is the result of the evolution of subgrains as they rotate relative to each other [100,112,113]. At the beginning of the process, the dislocation cells form cell blocks, which are separated by the dislocation sub-boundaries at misorientation angles much larger than those between adjacent cells. For cells and cell blocks, the misorientation angles are approximately $0.2\text{--}3^\circ$ and $4\text{--}13^\circ$, respectively [114,115]. In the course of deformation, the misorientation of cell blocks increases so that partial disclinations begin to form and move, which leads to the rotation of adjacent grain regions and the formation of new grain boundaries. Thus, the subdivision of original grains into smaller highly misoriented fragments occurs [14,113,116].

The ETMB model [28,63] considered here predicts the evolution of dislocation cell characteristics (cell sizes, dislocation densities inside cells and at cell boundaries) for each grain exposed to deformation. As noted in [64], “dislocation cell structure emerged during plastic deformation can be seen as a pre-cursor of the final grain structure to be formed at large strains, particularly under Severe Plastic Deformation”. From this point of view, the ETMB model provides a strong basis for constructing more detailed fragmentation models able to explicitly describe the formation of cell blocks and their rotations. On the other hand, the ETMB model, either in its original form or with a slight correction to the form of the equations, can also be used to simulate severe plastic deformation [50,65–67]. In this case, the above-mentioned processes are effectively taken into account when assessing the phenomenological dependences of the model parameters on the accumulated strain, which directly approximates the experimental data.

Each cell in the dislocation structure is represented by a composite two-phase structure [63]. The first phase is the “hard” cell walls, and the second phase is the “soft” cell interior. The idea that cells can be considered in this form was originally proposed in [117], where “hardness/softness” means the degree of dislocation motion obstruction; i.e., “hard” cell walls prevent slipping more strongly than “soft” cell interiors. Therefore,

the cell wall and interior are referred to as the regions with a high and low local dislocation density, respectively.

It should be noted that one of the main assumptions of the composite two-phase model [28] is that the dislocation cellular structure has already been formed. The question of how to describe the structure formation is discussed, for example, in [99,100,118,119]. Thus, the problems faced by researchers are as follows: identification of structural parameters via analysis of the experimental data (or the results of models describing the formation of a cellular structure) and description of the structure evolution caused by deformation.

In the ETMB model, an effective (average) cell whose parameters correspond to those averaged over all cells contained in the grain under study is considered. In the original model [63], the cell is in the shape of a cube with side l and wall thickness $w/2$; the initial value of l is determined by the initial value of dislocation densities in cell walls and cell interiors using the formulas given below.

The idea of the ETMB model is to describe the evolution of dislocation densities in cell interiors and cell walls and to determine the effective dislocation density using the rule of mixtures. The application of a phenomenological approach makes it possible to calculate the relation between cell size and dislocation density; acquiring a description of the change in cell size is one motivation for applying the ETMB model. Section 3.1 presents the relations of the original ETMB model, and Section 3.2 describes the modifications to the model relations used in this study. In the present work, the advanced ETMB model was embedded into a two-level CM, and new results were obtained for equal channel angular pressing of copper using the proposed mathematical apparatus (Section 4).

3.1. Relations of the Original ETMB Model

As noted above, the model under study assumes that the dislocation densities on all slip systems are the same, that is, $\rho^{(j)} = \frac{\rho}{K/2}$, where ρ is determined for a cell in accordance with the rule of mixtures. The dislocation densities in cell interiors and cell walls are denoted by ρ_c and ρ_w , respectively. Thus, we can write [63]:

$$\dot{\rho}_c = (\dot{\rho}_c)_{FR}^+ + (\dot{\rho}_c)_w^- + (\dot{\rho}_c)_{cs}^- \quad (5)$$

The first term in the right-hand part of (5) characterizes an increase in dislocation density in cell interiors, which occurs due to their generation by the Frank–Read source located near the cell walls [63]:

$$(\dot{\rho}_c)_{FR}^+ = \frac{\alpha^*}{\sqrt{3}} \frac{\sqrt{\rho_w}}{b} \dot{\gamma}_w, \quad (6)$$

where α^* is the constant characterizing the fraction of active sources of dislocation generation; $\dot{\gamma}_w$ is the shear rate occurring due to the dislocation motion in cell walls, which was defined by the Orowan equation $\dot{\gamma}_w = \rho_w b v_w$; and v_w is the average velocity of dislocation glide in cell walls. Note that (6) uses the shear rate for dislocations in cell walls. Based on [63] the Frank–Read sources near the cell walls induce dislocations both in cell walls and in cell interiors depending on the slip directions of dislocations activating these sources. Similarly, (11) uses the shear rate for dislocations in cell interiors to describe an increase in the dislocation density in cell walls.

The second term in the right-hand part of (5) characterizes a decrease in dislocation density in cell interiors, which occurs because some dislocations leave the cell interiors and move to the cell walls [63]:

$$(\dot{\rho}_c)_w^- = -\beta^* \frac{6\dot{\gamma}_c}{bl(1-f)^{1/3}}, \quad (7)$$

where β^* is the constant characterizing the fraction of dislocations leaving the cell interiors; $\dot{\gamma}_c$ is the shear rate occurring due to the dislocation motion in cell interiors, which was

defined by the Orowan equation $\dot{\gamma}_c = \rho_c b v_c$; v_c is the average velocity of dislocations glide in cell interiors [63]; and f is the cell walls volume fraction.

Finally, the third term in the right-hand part of (5) characterizes a decrease in dislocation density in cell interiors which occurs because of the annihilation of dislocations via cross-slip [63]:

$$(\dot{\rho}_c)_{cs}^- = -k_0 \left(\frac{\dot{\gamma}_c}{\dot{\gamma}_0} \right)^{-1/n} \dot{\gamma}_c \rho_c, \quad (8)$$

where k_0 is the constant; $\dot{\gamma}_0$ is the shear rate when the shear stress reaches its critical value; and n is the parameter which characterizes the strain rate sensitivity of annihilation process.

The relation describing the evolution of dislocation density in the cell wall ρ_w is taken as [63]:

$$\dot{\rho}_w = (\dot{\rho}_w)_{dep}^+ + (\dot{\rho}_w)_{FR}^+ + (\dot{\rho}_w)_{cs}^-. \quad (9)$$

The first term in the right-hand part of (9) characterizes an increase in the dislocation density in cell walls occurring due to the dislocations leaving the cell interiors [63]:

$$(\dot{\rho}_w)_{dep}^+ = \frac{6\beta^* \dot{\gamma}_c (1-f)^{2/3}}{b l f}. \quad (10)$$

The second term in the right-hand part of (9) characterizes an increase in the dislocation density in cell walls occurring due to the activation of the Frank–Read sources located near the cell walls and due to the motion of dislocations (induced by these sources) in the wall interior [63]:

$$(\dot{\rho}_w)_{FR}^+ = \frac{\sqrt{3}\beta^* \dot{\gamma}_c (1-f) \sqrt{\rho_w}}{f b}. \quad (11)$$

Finally, similarly to the third term in (5), the third term in the right-hand part of (9) characterizes a decrease in the dislocation density in cell walls which occurs because of annihilation [63]:

$$(\dot{\rho}_w)_{cs}^- = -k_0 \left(\frac{\dot{\gamma}_w}{\dot{\gamma}_0} \right)^{-1/n} \dot{\gamma}_w \rho_w. \quad (12)$$

By integrating relations (5) and (9), we can calculate the total dislocation density ρ for the cell as the weighted sum of dislocation densities in cell walls ρ_w and in cell interiors ρ_c [63]:

$$\rho = f \rho_w + (1-f) \rho_c. \quad (13)$$

A significant element of the model is the relation describing the evolution of the cell walls volume fraction f , which is introduced in terms of cell geometry [63]. It was shown in [63] that this relation was derived by analyzing the experimental results, and hence it can be calculated by the following empirical function [28]:

$$f = f_\infty + (f_0 - f_\infty) e^{-\gamma_r / \tilde{\gamma}_r}, \quad (14)$$

where γ_r is the scalar estimate of the accumulated shear strain on all SSs; f_0 is the initial value of the cell walls' volume fraction; f_∞ characterizes the saturation of f at large strains; and $\tilde{\gamma}_r$ describes the rate of cell walls volume fraction decrease.

Knowing the total dislocation density (13), the average cell size can be calculated using the following formula [63]:

$$l = \frac{K_r}{\sqrt{\rho}}, \quad (15)$$

where K_r is the proportionality parameter.

The validity of (15) has been proved by many experiments performed for different materials—pure iron [88], copper, iron–carbon and iron–silicon alloys [120], iron–nickel alloy [121] and pure nickel [95].

The relations given above demonstrate that the rate of cell size l change is dependent on the shear rates $\dot{\gamma}_c$ (in cell interiors), $\dot{\gamma}_w$ (in cell walls) and the integral estimate of shears γ_r .

As in [63], we also assume that the dislocation cells in a crystallite are identical, and the mechanical response can be characterized by the unique value of the shear rate $\dot{\gamma}_r$ which is taken to be the same for cell walls and for cell interiors (under Taylor's hypothesis):

$$\dot{\gamma}_w = \dot{\gamma}_c = \dot{\gamma}_r, \quad (16)$$

The value of $\dot{\gamma}_r$ is determined by the following relation [63]:

$$\dot{\gamma}_r = \left(\sum_{\alpha=1}^K \left(\dot{\gamma}^{(\alpha)} \right)^{(m_r+1)/m_r} \right)^{m_r/(m_r+1)}, \quad (17)$$

where m_r is the constant. The derivation of (17) is given in [63] and is based on the representation of the shear rate in the form of a power law viscoelastic relation, on the determination of the power in the entire crystallite by the sum of the powers for each slip system and on the assumption of isotropic hardening.

For each grain, the shear rates $\dot{\gamma}^{(\alpha)}$ over the slip system α is determined by means of the two-level statistical CM (Section 2).

3.2. Modifications of Some Relations of the ETMB Model Focused on Providing a More Accurate Description of Fragmentation

In the present work, we use the known modifications of some relations of the original ETMB model to provide a more accurate description of grain refinement from a physical point of view.

In [71], it was proposed that Equations (8) and (12), which describe the dislocation annihilation process, be changed into equations that take into account the magnitude of stacking fault energy (SFE) and temperature. It is known that annihilation is a thermally activated process [122] that depends the internal characteristics of the material such as degree of dislocation dissociation and rate of self-diffusion [123–125], which are determined by SFE magnitude [126]. It was shown in [127] that, when SFE decreases, the rate of dislocation annihilation in metals also decreases.

In the relations modified to describe the annihilation process, the key role is played by the cross-slip of screw dislocations for the dislocation density in cell interiors and the climb of dislocation dipoles for the dislocation density in cell walls. Note that the base CM does not account for the influence of screw dislocations on the material response because the screw dislocation density becomes rather small compared to the edge dislocation density at the early stage of deformation [128–130]; thus, when providing a comprehensive description of the material response, it is sufficient to account for the edge dislocations only.

However, in order to obtain a more accurate description of the dislocation processes in cells by means of the ETMB model, the screw dislocations must be taken into account. For this purpose, we use here the modifications to the original ETMB relations. It is important to note that the effect of screw dislocations on the material response is solely considered in the modifications of the ETMB model; the inelastic strain rate relation in (2a) is kept the same. The cross-slip of screw dislocations is described in terms of the Friedel–Escalaig model [131,132]. In order to predict the climb of dislocation dipoles, the diffusion processes are described by analyzing the velocity of jogs along dislocations [123,133]. Then the relations for describing the process of annihilation in cell walls and cell interiors are as follows [71]:

$$(\dot{\rho}_w)_{cs}^- = -B \exp\left(\frac{-U}{RT}\right) \left[\exp\left(\frac{\Omega_r \tau^*}{k_B T}\right) - 1 \right] \rho_w^2, \quad (18)$$

$$(\dot{\rho}_c)_{cs}^- = -\frac{Gb^4 v_D}{8\pi\Gamma V} \exp\left(-A \ln\left(\frac{Gb^4 v_D}{16\pi\Gamma V \dot{\gamma}_c}\right) + \frac{\tau_c V}{Gb^3}\right) \rho_c, \quad (19)$$

where $B = \frac{8\alpha b^2 v_D n_c}{\delta} \left(\frac{24\pi(1-\nu)}{(2+\nu)} \right)^2 \left(\frac{\Gamma}{Gb} \right)^2$; α is the material constant; v_D is the Debye frequency; n_c is the number of nearest neighboring sites for vacancy diffusion (for the FCC metals; n_c is approximately equal to 11 [123]); δ is the constant; ν is Poisson's ratio; Γ is the stacking fault energy; U is the self-diffusion activation energy; T is the temperature; R is the universal gas constant; Ω_r is atomic volume, τ^* is the stress acting on the leading dislocation in the dislocation pile-up during SPD, which can be estimated as [134] $2l\sqrt{\rho_w}\tau_w$, or approximated using (15) as $2K_r\tau_w$; τ_w is the critical shear stress in cell walls, calculated according to the equation [135] $\tau_w = \alpha Gb\sqrt{\rho_w}$; k_B is the Boltzmann constant; V is the activation volume for cross-slip; A is the constant; and τ_c is the critical shear stress in cell interiors defined by the relation [135] $\tau_c = \alpha Gb\sqrt{\rho_c}$. We remark that these relations explicitly describe SFE [71]. In fact, one of the priority directions of the development of multilevel crystal plasticity CMs is the construction of equations that can explicitly account for changes in intrinsic material parameters, such as SFE [136].

In addition, following [70,137] instead of the constant K_r , we will use in (15) a variable that decreases with an increase in the accumulated shear strain, as in the relation for the volume fraction of cell walls (14):

$$K_r = K_\infty + (K_0 - K_\infty)e^{-\gamma_r/k_r}, \quad (20)$$

where K_∞ characterizes saturation K_r at large strains, K_0 is an initial value K_r , k_r is the variation "rate" K_r . Relation (20) was constructed using the experimental data from [137]. The values of the constants K_∞ , K_0 , k_r were determined according to [137], but were changed to better fit the experimental data. The need to change them was caused by the differences in the models used in the current work (the two-level statistical model) and in [137] (the one-dimensional mechanism-based strain gradient plasticity model).

Thus, in this study, the following modifications of the ETMB model are applied: (18) and (19) are the equations to describe the annihilation process in cell walls and in cell interiors [71], and (20) is the equation for the constant K_r from (15) [70]. The introduced modifications seem to be a good basis for further in-depth description of the developed fragmentation process. Incidentally, it should be mentioned that in some studies, the original ETMB model was used to obtain an approximate description of grain refinement during severe inelastic deformations [63,65,68,74,76].

As can be seen from the above-mentioned relations, the CM and ETMB models are completely conjugated. According to (3), the CM hardening relations take into consideration the dislocation density and cell size calculated in the ETMB model. The relations given in Section 3 demonstrate that the shear rates for slip systems calculated by applying the CM model determine the rate of change in dislocation densities in the ETMB model.

The joint model is formulated in rate form. That is, in the CM, the SS shear rates $\dot{\gamma}^{(\alpha)}$ are determined, and (16) and (17) yield the values of $\dot{\gamma}_r$, $\dot{\gamma}_w$, $\dot{\gamma}_c$. In the ETMB model, the simulations performed using (5) and (9) yield the rate of change in dislocation densities in cell interiors ρ_c and cell walls ρ_w . Analysis of the current values of specified internal variables (IV) gives the values of total dislocation density (13), average cell size (15), and appropriate critical stresses (3).

In the numerical implementation, any integration scheme can be applied to the systems of ordinary differential equations. In our investigation, we use the Euler method. To integrate rotations, the instantaneous axis of rotation was determined and the rotation rate was integrated [6].

4. Results and Discussion

The approach proposed in this study uses a combination of the CM and ETMB models whose relations have been modified to provide an approximate description of grain refinement during equal channel angular pressing at room temperature. Recent experiments [77–80] demonstrated that, when ECAP is implemented at room temperature, recrystallization can be ignored. Therefore, recrystallization processes are not consid-

ered in the proposed model, which is consistent with the results obtained by other researchers [65,71,74,87,137,138].

Equal channel angular pressing is the multiple extrusion of a sample through a die containing two channels of the same area and cross-sectional shape which intersect at an angle Φ . When passing through the die, the sample experiences significant shear deformations while its shape remains unchanged, which allows any number of passes to be completed. In this paper, we consider the route B_C—the sample rotates by 90 degrees clockwise around its longitudinal axis during each pass. To model the ECAP process, the kinematic loading with a strain path change between passes was specified when setting a velocity gradient $\mathbf{L}(t)$ according to the algorithm derived in [78]. It should be noted that one of the advantages of multilevel models is their universality, namely, their applicability for the analysis of the processes of simple and complex loading with the same set of parameters [7,139].

Table 1 contains the values of the parameters used in the numerical analysis.

Table 1. Parameters of CM and modified ETMB for copper.

Parameter	Definition	Value
π_{1111} π_{1122} π_{1212}	independent components of the elastic property tensor [140]	168.4 GPa 121.4 GPa 75.4 GPa
$\dot{\gamma}_0^{(k)}$	viscoplastic relation (2b) parameter [139]	0.001 s ^{−1}
m	strain rate sensitivity exponent of the material [139]	50
$\tau_{c0}^{(k)}$	initial critical shear stress	10 MPa
α_{MHP}	modified Hall–Petch relation (3b) constant	0.02
G	shear modulus [72]	48 GPa
b	Burgers vector modulus [63]	2.56 Å
q_{lat}	latent hardening parameter [139]	2.0
α_{BH}	Bailey–Hirsch parameter	0.0132
α^*	constant that characterizes the fraction of active sources of dislocation generation [63]	0.065
β^*	constant that characterizes the fraction of dislocations leaving the cell interiors [63]	0.012
f_0	initial value of the volume fraction of cell walls [63]	0.25
f_∞	saturation of f at large strains [63]	0.06
$\tilde{\gamma}_r$	rate of cell walls' volume fraction decrease [63]	3.2
m _r	constant	250
α	material constant [63]	0.25
ν_D	Debye frequency [72]	10 ¹³ s ^{−1}
n_c	number of nearest neighboring sites for vacancy diffusion [72]	11
δ	constant [72]	5
ν	Poisson's ratio [72]	0.31
Γ	stacking fault energy [72]	45 mJ/m ²
U	self-diffusion activation energy [72]	203 kJ/mol
T	temperature	300 K
R	universal gas constant	8.31 J/(mol·K)
Ω_r	atomic volume [72]	b^3

Table 1. *Cont.*

Parameter	Definition	Value
k_B	Boltzmann constant	$1.38 \cdot 10^{-23}$ J/K
V	activation volume for cross-slip [72]	$300b^3$
A	constant	0.885
K_∞	numerical constants in (20)	9.5
K_0		30
k_r		4.0

Figure 1 depicts the dependence of the equivalent stress and the fraction of crystallites with a number of likely active slip systems on the equivalent strain during two ECAP passes on route B_C with an angle Φ of 90° at room temperature. The proximity to the activity of the slip system was determined according to [139]. For this purpose, the modulus of the difference between the shear stress and its critical value on it was calculated. If the estimated value was less than the value of some specified tolerance (5 MPa was used in the work), the system was considered likely to be active.

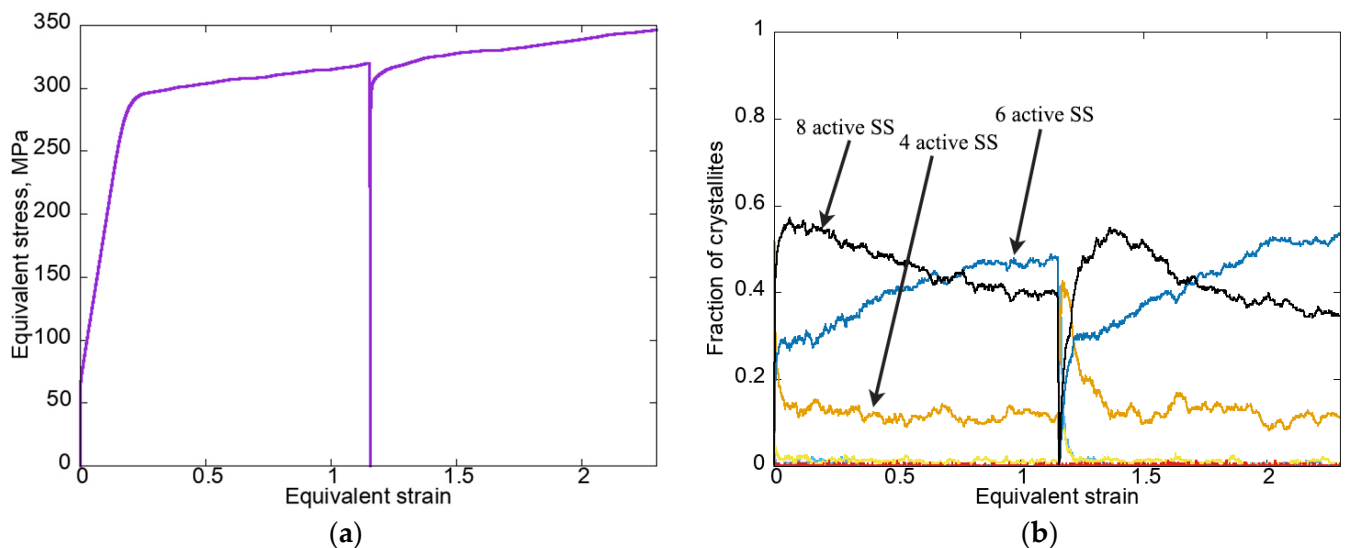


Figure 1. Dependences of (a) the equivalent stress and (b) the fraction of crystallites with a number of likely active slip systems on the equivalent strain of two ECAP passes on route B_C.

Note that the algorithm for finding likely active slip systems is useful for performing a statistical analysis of the mesostress motion along the crystallite yield surface in stress space, especially for loadings with a strain path change [139]. It is this analysis that allows a fairly simple and understandable explanation of the equivalent stress change on the stress–strain curve during loadings with a strain path change [139]. In Figure 1b, it is clear that, immediately behind the strain path change, the fraction of crystallites with four likely active slip systems is higher than the rest. This is reflected in the stress–strain curve by the equivalent stress drop observed after the strain path change. Note that it is impossible to compare the simulation results of the stress–strain curves in Figure 1a with the experimental data, because it is impossible to determine the flow stresses during ECAP experimentally. Therefore, in this article, as well as in the works of other researchers [37,72,74,137,138], a comparison of simulation results with experimental data on textures, yield stress and microstructure after different numbers of ECAP passes was performed, which is described below. At the same time, the results in Figure 1a show that it is possible to perform an analysis with simulations that would not be possible with experiments. In addition, the

model makes it possible to investigate in detail the evolution of the structure and the stress–strain state during the process locally, at different points of the billet under study.

In order to evaluate the influence of ECAP on the mechanical properties of the samples, the values of yield stress $\sigma_{0.2}$ obtained for the copper samples (pre-deformed by ECAP and subjected to quasi-uniaxial tension along their longitudinal axis Ox_1) are given in Table 2 for the modeling results and the experimental data [141]. The values of $\sigma_{0.2}$ were determined for different ECAP passes (the tension of the sample after 0 passes corresponds to as-received material) realized under the above conditions. Quasi-uniaxial tension here means a kinematic loading with the velocity gradient $\mathbf{L}(t) = \dot{\epsilon} \mathbf{p}_1 \mathbf{p}_1 - \frac{\dot{\epsilon}}{2} \mathbf{p}_2 \mathbf{p}_2 - \frac{\dot{\epsilon}}{2} \mathbf{p}_3 \mathbf{p}_3$, where $\mathbf{p}_i, i = \overline{1,3}$ is the LCS basis and $\dot{\epsilon}$ is the strain rate, s^{-1} . Note that this loading was proposed in [142] as an approximation of uniaxial loading for CM.

Table 2. Yield stresses for the copper samples subjected to quasi-uniaxial tension along their longitudinal axis Ox_1 (varying number of ECAP passes): modeling results and experimental data [141].

Pass Number	Yield Stress $\sigma_{0.2}$ (Model), MPa	Yield Stress $\sigma_{0.2}$ (Experiment), MPa
0	75.4	68 ± 6
1	345.6	342 ± 5
2	380.0	407 ± 22
4	436.4	415 ± 4

As one can see, the results of modeling are in strong agreement with the experimental data.

Figure 2 gives pole figures for the directions [111] (projection from the Ox_3 axis, where $Ox_1x_2x_3$ is the coordinate system related to the sample), obtained when modelling different numbers of ECAP passes. The initial orientation distribution was uniform.

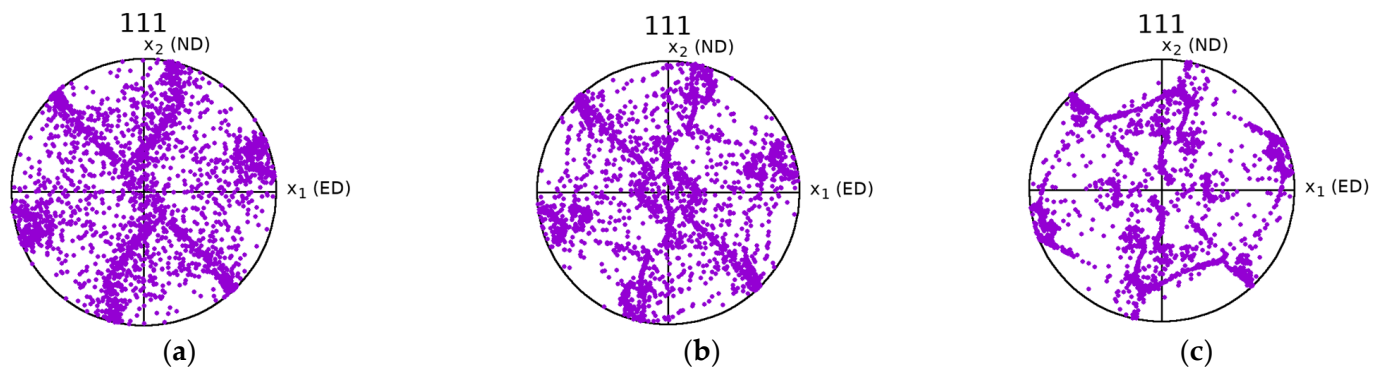


Figure 2. Pole figures for the directions [111] (a) by the end of the first pass, (b) by the end of the second pass and (c) by the end of fourth pass.

Figure 2 shows that the modeling results are in satisfactory qualitative agreement with the experimental data (see Figure 7 (B_C) in [78]). We note that the texture which appeared at the first pass retains its form during the second and subsequent passes, yet becomes more “acute”.

Figure 3 gives the dependences of the dislocation density in cell interiors and the average cell size on the equivalent strain (four ECAP passes), obtained using model calculations, as well as the experimental data [137]. The average cell size is determined by averaging the corresponding values over the number of crystallites in the RV.

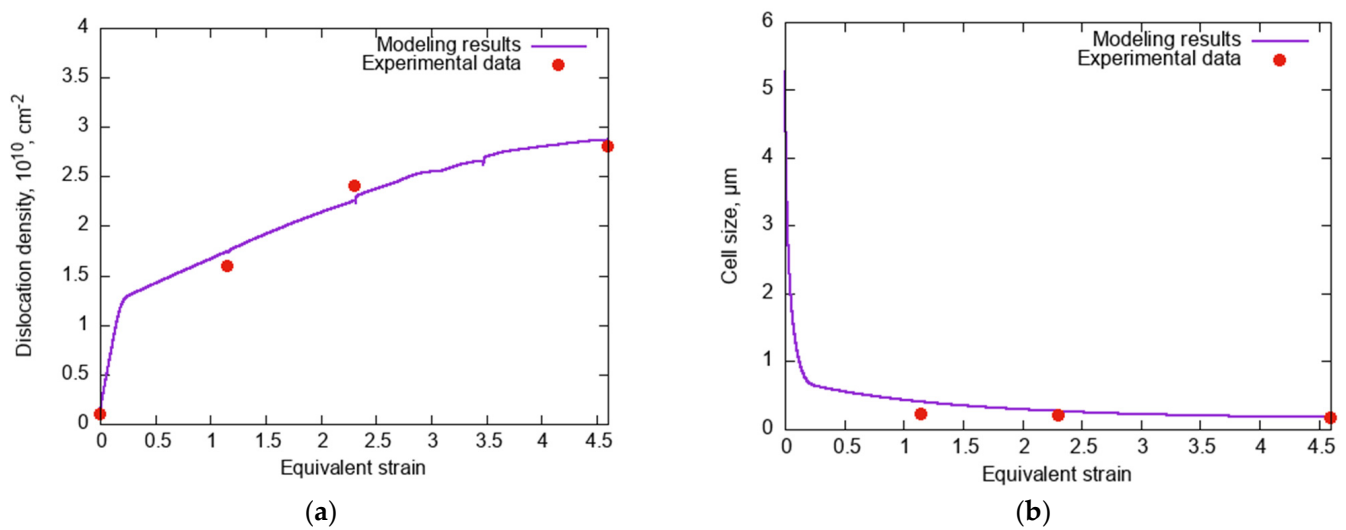


Figure 3. Dependences of (a) the dislocation density in cell interiors and (b) the average cell size on the equivalent strain (four ECAP passes), obtained using model calculations and the experimental data [137].

The modeling results shown in Figure 3 are in strong agreement with the experimental data [137], which indicates the ability of the developed model to describe the initial stage of fragmentation. The results for the dislocation density in cell walls are not given, since only the dislocation density in cell interiors was experimentally measured [137]. The dislocation density in cell walls was calculated using the relations of the proposed one-dimensional gradient macrophenomenological model with an integrated ETMB model.

When crystal plasticity CM and the ETMB model are used together, the distribution of the average cell size over crystallites can be analyzed. Figure 4 shows histograms with the fraction of crystallites that have an average cell size in a certain range after different numbers of ECAP passes. At the initial time moment, all crystallites have the same average cell size.

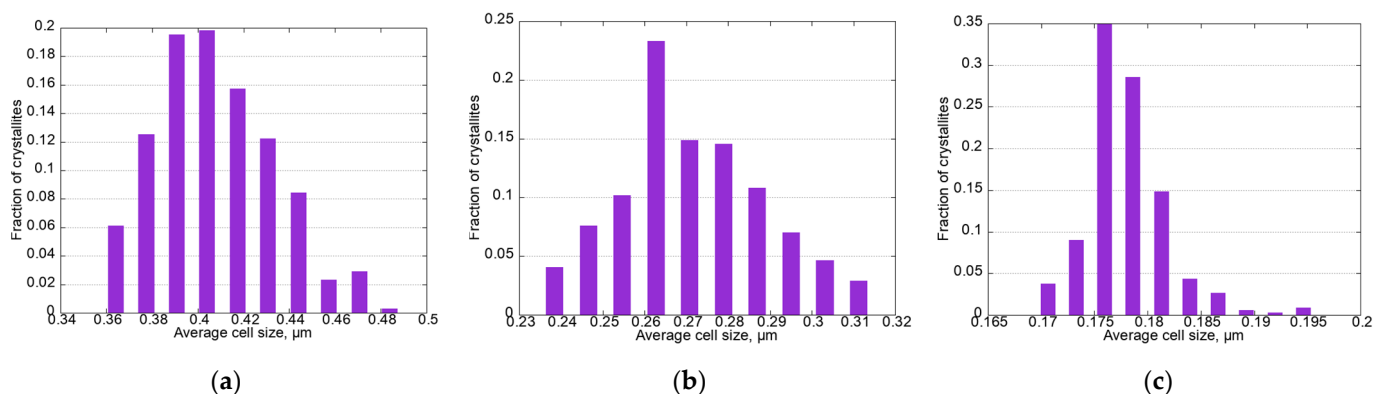


Figure 4. Histograms of average cell size distribution over crystallites (a) by the end of the first pass, (b) by the end of the second pass and (c) by the end of the fourth pass.

The results in Figure 4 qualitatively correspond to the lognormal distribution and agree with the experimental data [74]. The differences in the values of the average cell size in different crystallites are caused by the differences in the realization of IDS in them, since the average cell size depends on the integral estimate of the accumulated plastic shear. Note that the distribution dispersion decreases as the number of passes increases, which corresponds to the transformation of a coarse-grained polycrystal into a polycrystal with small equiaxed grains noted in the literature [50,66,72].

Thus, the results obtained using the two-level constitutive model with a modified ETMB submodel do not show complete quantitative agreement with the experimental data, which indicates a need for further development of the applied model. These relations should be used to determine the rates of change in the dislocation densities of cell interiors and cell walls for each slip system. This will make it possible to more correctly describe the material hardening and the grain structure refinement processes. The hardening law should also be modified so that it includes the grain size dependence according to the Hall–Petch relation. In order to obtain a description of developed fragmentation, it is necessary to analyze the process under study and to include an explicit description of the cell misorientation mechanism in the model. The problem is expected to be solved when geometrically necessary dislocations, whose density is associated with the misorientation angle of the cell boundaries, are explicitly considered in the model, as, for example, in the approach described in [143,144].

5. Conclusions

In this work, the ETMB submodel describing the evolution of average cell size under deformation was embedded into the two-level statistical constitutive model of FCC polycrystals. The original relations of the model and some of its modifications were considered to obtain an accurate, physically accepted description of the grain refinement process. In the paper, the constitutive model and the modified ETMB model were completely conjugated. The grain substructure characteristics from the ETMB model were taken into account in the hardening law. Numerical calculations were carried out using the constitutive model with an integrated modified ETMB submodel, which made it possible to consider the process of copper grain structure refinement during equal channel angular pressing at room temperature. The simulated results showed strong agreement with the experimental data.

Thus, it has been shown that the statistical crystal plasticity constitutive models can be applied in describing change in grain structure during severe plastic deformations. This indicates the possibility that these models can also be used to study and improve the technological processes of thermomechanical treatment of materials.

However, the constitutive model with an integrated ETMB submodel proposed in this paper needs to be improved. To obtain a clear description of the developed fragmentation, the mechanism of cell rotation should be explicitly described in the model. In the original ETMB and its modified version, this phenomenon is taken into account by the phenomenological dependences of the model parameters on the accumulated strain, which directly approximate the experimental data. Moreover, dislocation densities should be assessed separately for each slip system so that the grain structure refinement processes can be described adequately. It is also necessary to introduce an explicit description of grain size and to analyze grain size dependence in the hardening law according to the Hall–Petch relation. The model should also be able to describe the cell formation process, which is another acute problem.

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