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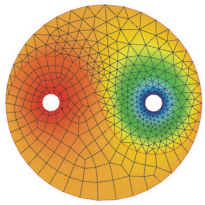

STRATEGIES OF TRANSPORT OF MICROSTRUCTURAL VARIABLES FOR REMESHING – APPLICATION TO TEXTURE-INDUCED MECHANICAL ANISOTROPY IN METALS

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Abstract

Finite element computations of metal forming often involve large deformations so that the mesh degenerates and a remeshing procedure is required. When microstructural variables are attached to the nodes or integration points of the mesh, they have to be transported from the old mesh to the new one by using an interpolation technique. Such interpolation of microstructure variables automatically induce numerical errors, and in many cases, may even have no physical meaning. In this paper two strategies of transport based on the Lagrangian particles concept are presented. They can be applied to a wide range of discretized microstructures. As an example, the transport of the variables of a polycrystalline plasticity model is used for simulations of uniaxial compression of a reference aluminium sample. Various numerical strategies are compared in terms of the accuracy of the description of the evolving mechanical anisotropy.

Key words: finite element, remeshing, microstructure, crystallographic texture, anisotropy

1. INTRODUCTION

In metal forming processes such as forging, the material experiences large plastic strains. If finite element simulations use a Lagrangian formulation, the mesh follows the material flow and it is distorted alike. Therefore, the initial mesh degenerates and a remeshing procedure is required in order to ensure numerical accuracy. Such a procedure implies the transport of state variables from the old mesh to the new one, which often proceeds using an interpolation method. Many of the state variables describe the evolving microstructure and are hence at the basis of the modelling of the mechanical behaviour. It is therefore important to check that the interpolation method has a physical meaning. This is, for example, not the case when crystallographic orientations are described using three Euler angles or when relying on a statistical sampling of grain sizes. In this work, we introduce and illustrate a novel way to transport such microstructural variables.

In the first part of this paper, the general framework of Lagrangian particles for the prediction of microstructure evolutions is recalled, and two strategies of transport of variables are described. In the next section, both strategies are applied to the transport of polycrystalline models variables. The appropriate number of Lagrangian particles to be used in a given mesh is discussed on the basis of predictions of the mechanical anisotropy. This analysis is per-

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formed considering different transport strategies and various numbers of remeshing operations. The final comparison allows identifying the most appropriate strategy.

2. STRATEGIES OF TRANSPORT OF MICROSTRUCTURAL VARIABLES USING THE CONCEPT OF LAGRANGIAN PARTICLES IN FINITE ELEMENT METHOD

The method is first presented without relying on specific characteristics of a microstructure in order to show the wide range of potential applications. We assume however that a discrete representation of the microstructure is available, and that a coupling between mechanical and microstructural evolutions can be computed within the framework of the finite element technique.

Let us consider a description of a representative microstructure consisting of N phases. Each phase is characterized by k scalar, vector or tensor variables describing its physical attributes. Geometrical properties can be quantified through shape functions depending on d characteristic lengths and a characteristic angles. A topological description can also include correlation functions, giving the probability to find neighbouring points at some distance of one another, in order to display different physical or geometrical properties. Each of these functions is assumed to be described by Γ variables. Therefore, in this approach, the global description of the microstructure within a representative volume of material requires $N_v = N(k+d+a)+\Gamma$ variables.

In the following, we will assume no topological description, that is to say no correlation functions between the phases. Only the volume fraction of each phase is taken into account, so that $\Gamma = N$.

In a 'classical' approach meant to compute microstructure evolutions with a finite element method, a complete representation of the discretized microstructure of N phases is usually considered at each integration point, and a homogenization technique is used to predict the mechanical behaviour and the microstructure evolution. During the simulation, the microstructure evolves according to the local deformation path, which is different from one integration point to another.

When the finite element mesh degenerates, that is to say when the distortion of the elements induces inappropriate Jacobian values, remeshing is needed, and state variables must be transferred from the old mesh to the new mesh (Coupez, 1991). Distribution functions of microstructural variables usually cannot be transported using classical spatial interpolation. For example, the conservation of the distribution functions of phase volume fractions during remeshing is problematic since there is neither a bijection nor a simple inclusion relationship between the set of distribution function parameters associated to the integration points of the old mesh and the corresponding set for the new mesh.

We propose here a method that is based on a new spatial mapping of microstructural information according to volume divisions which are different from the finite elements. The goal is to conserve the physics-based information through remeshing events.

The principle consists in distributing particles over a volume, as illustrated in Figure 1 in the case of a cylinder. Only one eighth of the cylinder is represented because of the symmetry of the microstructure and uniaxial compression. The particles are defined by their initial positions in the cylinder. These particles are Lagrangian particles in the sense that, when the volume is deformed, they follow the material flow, and the mesh in the case of a Lagrangian finite element formulation (see Figure 1). Contrary to integration points, these particles are neither displaced, nor removed, during remeshing events and can be considered as actual material points.

A cell is defined for each particle as the set of integration points which are closer to this particle than to any other particle, using the usual Euclidean distance definition (see Figure 1 b where two cells are sketched).

The complete representation of the sampled microstructure is associated to each particle. At a given time, a cell can be defined for a given particle. Within this cell, the representative microstructure associated to corresponding particle is distributed among the different integration points of the cell. Each phase of the sampled microstructure is associated to a single integration point of the cell, together with its (k+d+a+1) variables. But the selection of the particular integration point within the cell to which each phase is associated is random.

When the constitutive laws are based on microstructural variables, and since the mechanical behaviour is typically calculated at each integration point, the sum of the volume fractions of the phases attributed to an integration point should be proportional to the volume associated to this integration point (see

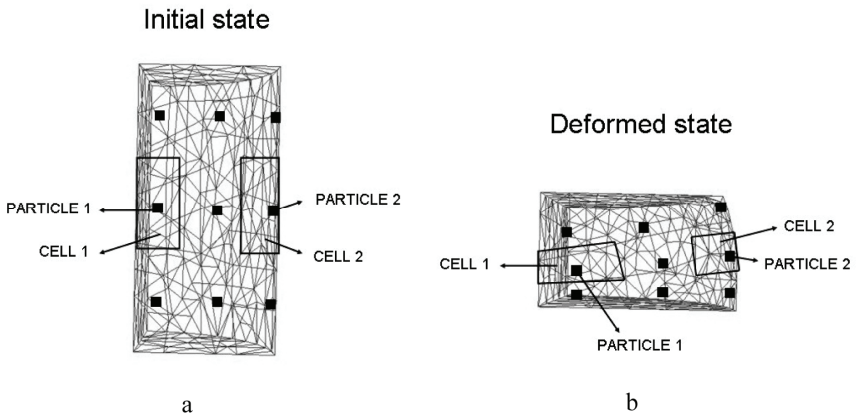

Figure 1. Initial and final configurations (a and b respectively) of one eighth of a cylinder under uniaxial compression. Lagrangian particles are designated by black dots. The evolution of two cells is sketched in the deformed state (b).

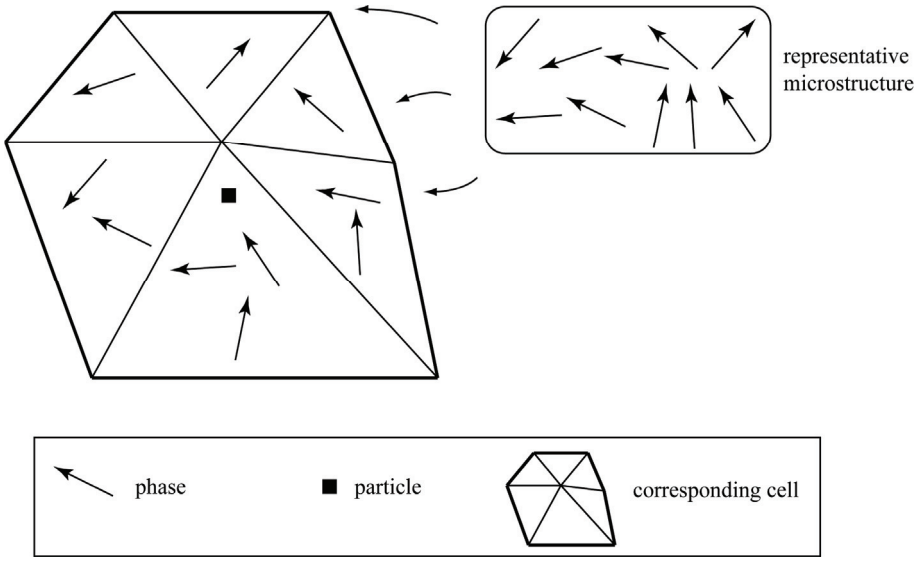

Figure 2. Illustration of the distribution of a sampled microstructure within one cell, assuming that each finite element contains a single integration point.

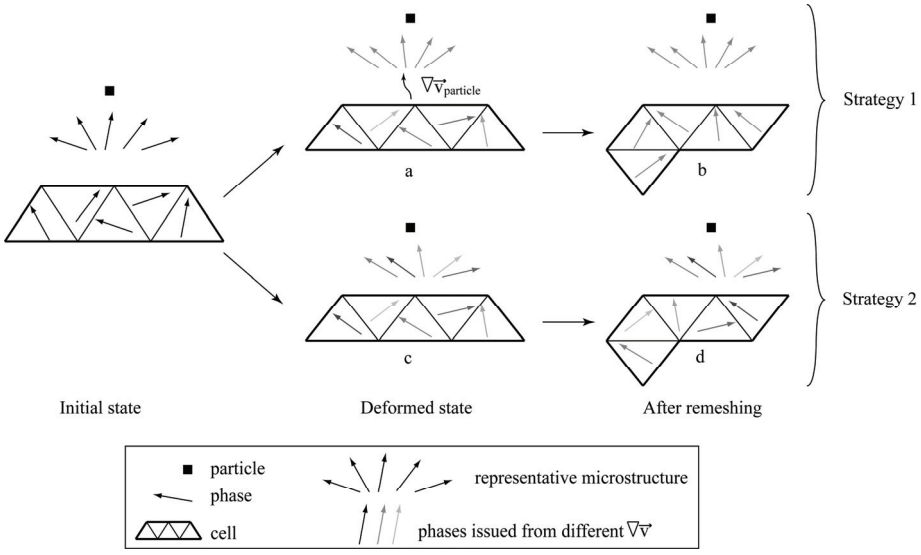

Figure 3. Illustration of the two strategies of microstructural variables transport in the case of one cell assuming that finite elements contain one single integration point each. Strategy 1 (a : calculation of the phase evolution, b : remeshing), strategy 2 (c : calculation of the phase evolution, d : remeshing).

Figure 2). Further details of these conditions and related numerical solutions can be found in (Béringhier, 2006; Béringhier *et al.*).

When remeshing occurs, particles are conserved, but new cells have to be identified on the basis of the positions of the integration points within the new mesh. Transport of the state variables simply proceeds by randomly redistributing the phases associated to a particle among the integration points of the new cell. From a physics point of view, this operation is acceptable if each cell spans a "sufficiently homogeneous" area in terms of deformation fields. Particles must therefore be adequately located throughout the mesh.

Sometimes, the microstructure evolution is highly sensitive to strain path. Then, the state variables may evolve differently depending on whether one considers the strain path computed at the integration point or the strain path averaged over the cell. This observation is at the basis of the two strategies proposed hereunder.

In strategy 1, the velocity gradient of the particle is computed as the average of the velocity gradients at the integration points of the cell. The history of the averaged velocity gradient is recorded until the next remeshing operation occurs. When remeshing is required, one recalculates the evolution of all state variables associated to a given particle according to the history of the average velocity gradient (Figure 3 a). In other words, all phases are now assumed to have evolved according to a common velocity gradient.

Therefore, the state variables within a cell are not conserved through remeshing events (Figure 3 b).

In strategy 2, the microstructure of a particle is simply considered as the union of the phases associated to the integration points of the cell. Each phase is subjected to a different history of the velocity gradient and state variables are conserved through remeshing events (Figure 3 c and d).

3. APPLICATION TO THE TRANSPORT OF POLYCRYSTALLINE MODELS VARIABLES

A classical example of finite element simulation of metal forming that is coupled with microstructure evolution is the prediction of the anisotropy induced by the crystallographic texture. For such numerical simulations, the microstructure is described by a crystallographic texture which is itself represented by a discrete set of orientations or 'representative grains'. These representative grains can be considered as phases in the formulations described in this paper. Homogenization schemes based on crystal plasticity theory allow computing the mechanical anisotropy of the metal from the crystallographic texture and some state variables of the single crystal (Taylor, 1938; Lebensohn *et al.*, 1993; Lebensohn *et al.*, 2005). They account for strain-induced texture evolution and predict the evolving mechanical anisotropy during metal forming operations. The strategies of transport proposed above are applied to this class of simulations in the following sections.

3.1. The finite element model and the simulations features

In this study, simulations are performed with Forge3® finite element code. This code used a mixed velocity-pressure formulation and the P1+/P1 tetrahedral mini-element (Aliaga, 2000). The polycrystalline model considered is an elastic-viscoplastic Taylor model. The crystal plasticity algorithm of this model can be found in (Delannay *et al.*, 2006). Microstructural variables are attached to each representative grain: 3 Euler angles describing the crystallographic orientation, the critical resolved shear stresses of potentially active slip systems, and the stress tensor acting on the crystal. In the simulations presented here, the initial stress is assumed to be negligible, that is to say that it is assumed that the material contains no initial internal stresses. The initial texture is measured on a 7582 aluminium alloy rolled at 70% thickness reduction (Figure 4). This texture is discretized into 1200 crystallographic orientations with identical volume fractions (Melchior and Delannay, 2006). The constitutive law is described at the level of a grain, that is to say at the level of a single crystal. For FCC metals, crystallographic slip may be modelled with 12 slip systems {111}<100>. The initial critical resolved shear stress τ_{c0} is assumed to be identical for the 12 slip systems and is set to 0.1 GPa. Elastic constants are given as follows : $C_{11} = 107.3$ GPa, $C_{12} = 60.9$ GPa, $C_{44} = 28.3$ GPa. Dislocation slip rates are calculated based on a viscoplastic exponential law:

$$\dot{\gamma} = \dot{\gamma}_0 \left| \frac{\tau}{\tau_c} \right|^{1/m} sign(\tau) \tag{1}$$

where $\dot{\gamma}$ is the dislocation slip rate, τ_c the critical resolved shear stress, τ the resolved shear stress, $\dot{\gamma}_0 = 0.001$/s a characteristic slip rate and m = 0.02 the strain rate sensitivity.

The hardening law is a Voce law:

$$\dot{\tau}_c = H_0 \left(\frac{\tau_{sat} - \tau_c}{\tau_{sat} - \tau_0} \right) \sum_{\beta} \left| \dot{\gamma}^{\beta} \right| \tag{2}$$

where τ_{sat} is the stress at saturation and H_0 the hardening parameter. τ_{sat} is set to 0.3 GPa and H_0 to 0.03 GPa.

The simulated test is a uniaxial compression test of the cylindrical specimen with friction, which induces a non homogeneous material flow. The operating conditions are:

$$v = 1 mm.s^{-1}, \varepsilon = 60\%,$$

where v is the press velocity and ε the engineering strain.

The friction between the cylindrical sample and the tools will induce a barrelling of the sample, and the strain heterogeneity throughout the deformed sample. The friction law is taken as a Tresca law:

$$\tau = \overline{m}\, \sigma_0 / \sqrt{3} \tag{3}$$

with a Tresca friction coefficient $\overline{m}$ of 0.3.

The mesh is based on the cylindrical shape of the samples, and the symmetries observed in the experimental pole figures and in the loading conditions allow dealing with only 1/8 of the cylinder, that is to say a pie of 50 mm in external radius and of 100 mm

in height which is discretized into 1085 finite elements. The initial sampled texture is then distributed 66 times in the mesh. This number is set so as to have enough crystallographic orientations per integration point to respect the proportionality between the sum of the volume fractions of the phases associated to an integration point and the volume of this integration point as mentioned above and explained in (Béringhier, 2006).

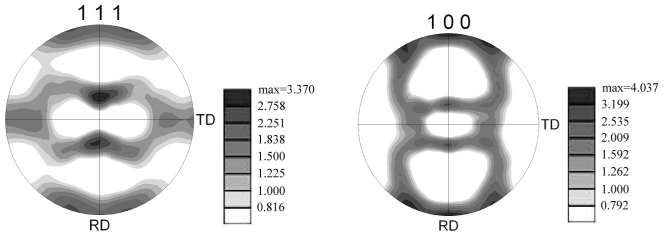

Figure 4. Initial texture of a 7582 aluminium alloy rolled at 70%.

In practice, no remeshing would be needed for such a test case since finite elements are not significantly distorted, but for our fundamental study and the thorough analysis of the different strategies, remeshing events may be artificially triggered at a controlled frequency. One simulation refers to the case when the classical approach is used, with one initial texture at each integration point, and no remeshing event is triggered at any stage of the compression. It could therefore be considered as a 'reference simulation'.

And the two transport strategies are tested for triggered periodic remeshing events. They are referred to as simulation 1 and simulation 2 for strategies 1 and 2 respectively.

The performance of the two simulations is discussed in terms of the accuracy of the mechanical anisotropy prediction. For uniaxial compressions of a cylinder with an orthotropic crystallographic texture, the final shape of the cross-section becomes an ellipse. The anisotropy of the material flow is described with the ovaling rate, OV, which is defined as follows:

$$OV = \frac{L\max - L\min}{L\min} \tag{4}$$

where Lmax and Lmin are the lengths of two axes of an elliptic transverse cross-section of the sample. Of course, due to friction, this ovaling rate is different at different height along the longitudinal axis of the sample, and it evolves as the compression proceeds.

3.2. Results and discussion

Various simulations are performed in order to study: (a) the transport strategies (b) the number of particles in the mesh, and (c) the number of remeshings during numerical compression test.

First, simulations with a single particle in the mesh and 5 remeshing events are analysed. The predictions for the final deformed state in terms of transverse cross-section ovaling rates at different heights along the longitudinal axis of the sample are reported in Figure 5. The height of 0 mm corresponds to the middle height of the cylinder, while the maximum height of the deformed final state is 40 mm since the engineering strain value reaches 60%.

For the 'reference' simulation, the ovaling rate decreases with the height. For test simulations with strategies 1 and 2 used at triggered remeshing events, the trend is completely different. These incorrect results can be explained as follows:

- in strategy 1, the distributed orientations are issued from an average velocity gradient which does not take into account the strain heterogeneity in the whole volume
- in strategy 2, the orientations are spread and mixed over the whole volume. When they are assigned to highly deformed areas, then they evolve. When they are assigned to areas which are hardly deformed, they will not evolve significantly. Therefore, after several remeshing operations, the texture tends to be similar to that of the highly deformed areas.

As expected, a minimum number of particles is needed in order to obtain an appropriate texture gradient description.

Then, the influence of the number of particles is studied by comparing simulations with 27 and 48 particles in the mesh, and 5 remeshing events during the simulation of the whole test. Satisfactory results for the ovaling rate are obtained with both transport strategies, as shown in Figure 6. The results tend towards those of the reference case as the number of particles is increased. Indeed, when the number of particles is increased in the mesh, the cell size is automatically decreased and the redistribution of polycrystalline variables is performed over smaller areas which are systematically less heterogeneous in terms of strain. The deformation gradients are therefore better captured and discretized spatially. And since the information in terms of texture evolution is concentrated in areas with more homogeneous strains, the induced mechanical anisotropy is better predicted.

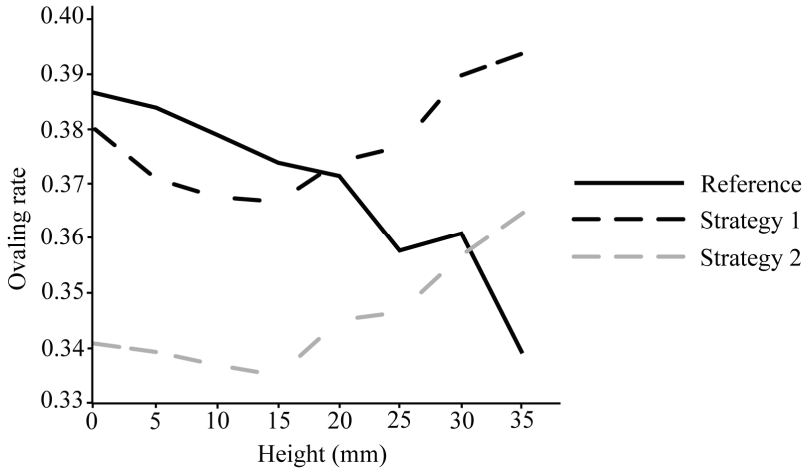

Figure 5. Ovaling rate at different heights of the specimen for the deformed final state in the case of one particle and 5 remeshings.

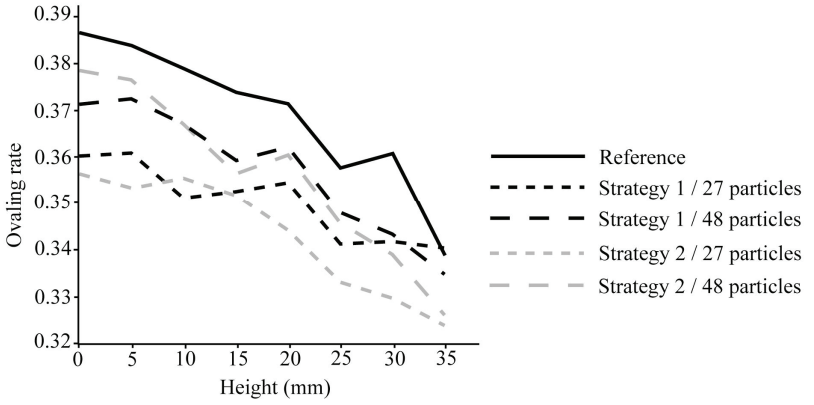

Figure 6. Ovaling rate at different heights of the specimen for the deformed final state in the case of 27 and 48 particles with 5 remeshings.

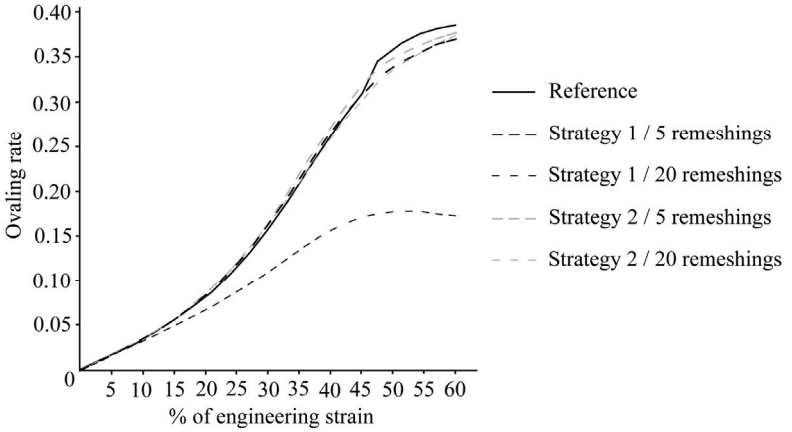

Figure 7. Evolution of the ovaling rate at middle height with the engineering strain in the case of different number of remeshing 5 and 20 and 48 particles in the mesh.

Finally, the effect of the number of remeshing events is investigated for both strategies. A total of 48 particles are set in the mesh, and simulations of the same test are done with 5 and 20 remeshing events respectively. The evolution of the ovaling rate at mid-height of the sample as the deformation proceeds is plotted in Figure 7. Strategy 1 is found to give satisfactory results with 5 remeshings, but when 20 remeshings are triggered, the ovaling rate starts diverging after an engineering strain of 10%, i.e. after 3 remeshings. Simulations were also performed for larger numbers of particles, and it is found that, with less than 128 particles in the mesh, non satisfactory results are obtained with strategy 1. Strategy 2 gave satisfactory results with both numbers of remeshing events.

4. CONCLUSION

Two generic strategies for the transport of microstructural variables during remeshing have been applied to finite element simulations of compression of a textured specimen. Detailed investigations have dealt with the specific cases when microstructural variables include crystallographic texture features. These transport strategies have been constructed so as to calculate more precisely the evolution of the different phases or grains with respect to velocity gradient (strategy 1), or the conservation of the exact description of these phases (strategy 2). From the comparison of their respective sensitivity to the number of particles in the mesh and to the number of remeshings during a deformation process, one can conclude that the conservation of the phases is more critical to obtain accurate results after a large number of remeshing events. Indeed, robustness with respect to the number of remeshings is fundamental since, for simulations with automatic remeshing, many remeshing events might be needed.

This methodology and these strategies can also be applied to other types of microstructural variables which cannot be interpolated by using classical transport techniques, for example when one models grain size distributions.

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STRATEGIE PRZESYŁANIA PARAMETRÓW MIKROSTRUKTURY PRZY AKTUALIZACJI SIATKI (REMESHINGU) – ZASTOSOWANIE DO MECHANICZNEJ ANIZOTROPII W METALACH WYWOŁYWANEJ TEKSTURĄ

Streszczenie

W obliczeniach metodą elementów skończonych często mamy do czynienia z dużymi odkształceniami siatki i wymagana jest jej aktualizacja (remeshing). Jeżeli w punktach całkowania lub w węzłach określone są parametry mikrostruktury, muszą one zostać przeniesione ze starej siatki do nowej. Stosowane są w tym celu metody interpolacji. Interpolacja zmiennych opisujących mikrostrukturę wprowadza błędy numeryczne i, w wielu przypadkach, może nie mieć fizycznego znaczenia. W pracy przedstawiono dwie strategie przekazywania oparte na idei cząstek Lagrange'a. Metody te mogą zostać zastosowane do szerokiego zakresu dyskretyzowanych mikrostruktur. Przeniesienie zmiennych modelu krystalicznej plastyczności zastosowano do symulacji osiowosymetrycznego ściskania próbki z aluminium przedstawiono w pracy jako przykład. Różne strategie numeryczne są porównane odnośnie dokładności opisu rozwijającej się w materiale mechanicznej anizotropii.

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