Simulation of meso–macro dynamic behavior using steel as an example

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Abstract

Presented in this paper is a model, where strain hardening and strain rate sensitivity are taken into account. The cellular automata rules are included into a continuum mechanics formulation to describe shear band propagation at the mesoscale. We apply the model in simulating deformation of the 20MnMoNi55 steel as an example. The macro stress–strain behavior and plastic strain patterns at the mesolevel are analyzed in the course of a computational tension test. © 2003 Elsevier B.V. All rights reserved.

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1. Introduction

Nowadays, consideration of plastic deformation as a process that develops at different scale levels is the most important and intensively discussed problem in physics and mechanics of solids [1,2]. Attributed to theoretical and computational methods, the essence of this problem can be formulated as reviewing basic conventional approaches to current understanding of plastic flow: continuum mechanics and discrete dislocation theory [1–3]. Each of them gives us a correct solution to a certain problem but needs to be developed for an adequate description of complex mechanical behavior of a heterogeneous material. One way of doing so is to involve into these formulations a length scale in an explicit or implicit form [2]. The second way we have been developing is to introduce the initial material structure in an explicit form into a continuum-mechanics consideration. Earlier, the latter approach was applied in numerical simulation of localized deformation in mesovolumes of polycrystalline materials as well as dynamic processes, including shock wave loading and ultrasonic surface treatment [1,3–5]. This allows us to investigate numerically the influence of structural parameters (size and quantity of grains, shape of interfaces, different types of inclusions and coatings, stress concentrations, etc.) on mesoscale stress–plastic strain pattern and macro stress–strain behavior for the certain materials. However, the problems connected with the shear-band origination and propagation were
disregarded because we used a conventional averaged formulation of the problem.

The main aim of this work is to present a comprehensive model, where the following effects are taken into account.

- We introduce some special rules from the discrete cellular automata method into a continuum mechanics formulation and carry out test calculations under dynamic loading [6,7]. In this way we can simulate low speed processes at the mesoscale. In this paper we apply the rules to modeling Luders band propagation (LBP).
- Quadratic function is used to simulate strain hardening.

Relaxation constitutive equation including the time dependence in an explicit and implicit form is applied to take strain rate sensitivity into consideration.

To illustrate the model, we simulate mechanical behavior of a steel specimen under tension.

2. Mathematical formulation

To investigate both macro stress–strain behavior and plastic strain pattern at the mesolevel, we used the system of equations of solid mechanics for plane stress. The mesoscopic deformation processes were simulated within a two-dimensional formulation of the problem. Numerical solutions were performed in terms of Lagrangian variables using the finite-difference method.

2.1. Basic equations

Stress tensor components \( \sigma_{33}, \sigma_{13}, \) and \( \sigma_{23} \) are assumed to be zero in the case of plane stress

\[
\sigma_{33} = \sigma_{13} = \sigma_{23} = 0, \tag{1}
\]

so the equations of motion take the form

\[
\sigma_{11,1} + \sigma_{21,2} = \rho \ddot{u}_1, \quad \sigma_{12,1} + \sigma_{22,2} = \rho \ddot{u}_2, \tag{2}
\]

where \( \rho \) is the mass density, \( u_1 \) and \( u_2 \) are the displacement vector components, the upper dots denote time derivatives and the commas in the subscripts denote space derivatives.

For independent components of the total strain rate tensor we can write the following expressions:

\[
\dot{\varepsilon}_{11} = \dot{u}_{1,1}, \quad \dot{\varepsilon}_{22} = \dot{u}_{2,2}, \quad \dot{\varepsilon}_{12} = \frac{1}{2} (\dot{u}_{1,2} + \dot{u}_{2,1}) \tag{3}
\]

and, using (1), the third component can be written as

\[
\dot{\varepsilon}_{33} = \dot{u}_{3,3} = - \frac{v}{1 - v} (\dot{u}_{1,1} + \dot{u}_{2,2}). \tag{4}
\]

Here \( v \) is Poisson’s ratio.

Assuming (3) and (4), the conservation law takes the form

\[
\dot{\rho} + \frac{1 - 2v}{1 - v} \rho \cdot (\dot{u}_{1,1} + \dot{u}_{2,2}) = 0, \tag{5}
\]

A constitutive equation is needed to close the system of Eqs. (2)–(5). Taking into account the decomposition of the stress tensor into the spherical and deviatoric parts \( \sigma_{ij} = -P \delta_{ij} + S_{ij} \), and assuming elastic strain to be the difference between the total and plastic strains \( \varepsilon_{ij}^e = \varepsilon_{ij} - \varepsilon_{ij}^p \), we obtain for non-zero stress tensor components

\[
\dot{S}_{11} = 2\mu \left( \dot{\varepsilon}_{11} - \frac{1}{3} \dot{\varepsilon}^{pp}_{kk} - \dot{\varepsilon}^{pp}_{11} \right), \tag{6}
\]

\[
\dot{S}_{22} = 2\mu \left( \dot{\varepsilon}_{22} - \frac{1}{3} \dot{\varepsilon}^{pp}_{kk} - \dot{\varepsilon}^{pp}_{22} \right), \tag{7}
\]

\[
\dot{S}_{12} = 2\mu \left( \dot{\varepsilon}_{12} - \dot{\varepsilon}_{12}^p \right), \quad \dot{S}_{33} = \dot{P} = -K \dot{\varepsilon}_{kk}. \tag{8}
\]

Here \( K \) and \( \mu \) are the bulk and shear moduli, respectively, and \( \delta_{ij} \) is the Kronecker delta.

2.2. Strain hardening, mesoplastic flow, and relaxation

One of the most important problems is to correctly define the plastic strain rate tensor in (6). This is dictated by the necessity to adequately describe mechanical behavior for different materials that could be subjected to different types of loading.

Firstly, we should incorporate strain hardening in the constitutive equations. To do so, we can write the rule for every local region of material as

\[
\sigma_{\text{eff}} = f(\varepsilon_{\text{eff}}^p), \tag{8}
\]
Eq. (8) is a classical macroyield criterion. This rule alone is not enough to simulate shear band propagation at the mesolevel because the material sound velocity limits the specific speed of a process in dynamic formulation. To solve the problem, we modify the classical force criterion by adding special rules from the cellular automaton method [8]. Following this approach, plastic deformation can develop according to (8) only in the local regions that lie near interfaces. We assumed any local region inside a material volume to be plastically deformed, provided specific plastic strain intensity reaches its critical value in one of the nearest local regions

\[ \varepsilon_{\text{eff}}^p = \varepsilon^* \]  

in any nearest local region (9)

where \( \varepsilon^* \) is the model parameter that reflects material properties at the mesoscale.

Thus, for the regions near the interfaces, the yield criterion covers rule (8), and for other regions—rules (8) and (9). This allows us to prescribe for plastic deformation to gradually propagate through material in a step-by-step mode at a certain physical velocity lower that that of sound.

In the case of plane stress we have for effective values

\[ \sigma_{\text{eff}} = \frac{1}{\sqrt{2}} \left\{ \left( S_{11} - S_{22} \right)^2 + \left( S_{22} - P \right)^2 \right. \]

\[ \left. + \left( P - S_{11} \right)^2 + 6 S_{12}^2 \right\}^{1/2} \]  

\[ \varepsilon_{\text{eff}}^p = \frac{\sqrt{2}}{3} \left\{ \left( \varepsilon_{11}^p - \varepsilon_{22}^p \right)^2 + \left( \varepsilon_{22}^p - \varepsilon_{33}^p \right)^2 \right. \]

\[ \left. + \left( \varepsilon_{33}^p - \varepsilon_{11}^p \right)^2 + 6 \varepsilon_{12}^p \right\}^{1/2} \]  

where \( \varepsilon_{ij}^p \) and \( \varepsilon_{ij} \) are the strain rate and stress tensor components, respectively.

Let us note that by assuming plastic strain rate to be in proportion to a scalar parameter, we can implement the procedure for stress correction with respect to the yield surface (8). In this case we would obtain quasistatic behavior only.

To incorporate strain rate sensitivity into the model, let us consider the plastic flow theory rule [9] associated with criterion (8):

\[ \dot{\varepsilon}_{ij}^p = \frac{3}{2} \frac{\dot{\varepsilon}_{ij}^p}{\sigma_{\text{eff}}} \sigma_{ij} \]  

Substituting the viscous relaxation model defining the effective plastic strain rate [5] into (12), we obtain for the plastic strain rate tensor

\[ \dot{\varepsilon}_{ij}^p = \frac{1}{2\eta} \left( 1 - \frac{f(\varepsilon_{\text{eff}}^p)}{\sigma_{\text{eff}}} \right) S_{ij}, \]  

where \( \eta \) is the relaxation factor. Eq. (13) means that all stress components (6) and (7) relax in a similar fashion.

In the work presented, we simulate the mechanical behavior of steel at average strain rates up to \( 10^3 \) s\(^{-1} \). In this case, there is no necessity of using a complex dependence for \( \eta \), contrary, for instance, to the shock wave loading [5,7], where the strain rates can exceed \( 10^7–10^8 \) s\(^{-1} \). We offer here two different simple relations

\[ \eta = A \sigma_{\text{eff}} + B \dot{\varepsilon}_{\text{eff}}^p, \] \[ \eta = A' \sigma_{\text{eff}} + B' t, \]

the second prescribing for the plastic strain rate to depend on time \( t \) in an explicit form. Here \( A, A', B, \) and \( B' \) are constants and are explicitly given in Section 3.

### 2.3. Initial and boundary conditions

Let us consider region \( A(x,t) \) with boundary \( BC(x,t) \), where \( x \) is the radius-vector. Zero initial conditions at \( t = 0 \) are set for all \( x \in A(x,0) \) (Fig. 1):

\[ \dot{u}_i(x) = 0, \quad \sigma_{ij}(x) = 0, \quad \rho(x) = \rho^{(0)}(x). \]  

The boundary conditions take the form

\[ \dot{u}_1(x,t) = -U = \text{const} \quad \text{for} \ t \geq 0, \ x \in BC1, \]

\[ \sigma_{ij}(x,t) \cdot n_j = 0 \quad \text{for} \ t \geq 0, \ x \in BC2, \]  

![Fig. 1. Schematic of the region under calculation.](image-url)
\[ \dot{u}_2(x, t) = 0 \quad \text{for} \quad t \geq 0, \quad x \in BC3, \]
\[ \dot{u}_1(x, t) = 0 \quad \text{for} \quad t \geq 0, \quad x \in BC4, \]
where \( n_j \) are the vector components normal to the surface, \( BC = BC1 \cup BC2 \cup BC3 \cup BC4 \).

### 3. Calculation results

All calculations presented in the work were carried out for the 20MnMoNi55 steel as an example. For this type of steel, there are following values of the material parameters: \( \rho^{(0)} = 7.9 \ g/cm^3; \mu = 90 \ GPa; \) and \( K = 145 \ GPa \). Stress in the figures is simulated as the average effective stress throughout the region \( A(x, t) \) in accordance with the following relation:

\[
\left\langle \sigma_{\text{eff}} \right\rangle = \frac{\sum_k \sigma_{\text{eff}}^k V^k}{\sum_k V^k}, \quad (18)
\]

where \( k \) denotes the number of a computational-grid cell and \( V^k \) is the current volume of this cell. We assign for the strain in the figures to be a relative elongation of the testpiece in direction \( x_1 \) (refer to Fig. 1).

The main novelty of the model proposed is the introduction of a modified plasticity criterion into consideration. It is assumed that the outset of plastic flow in a local region depends not only on its stress–strain state parameters but also on those in the adjacent material. This statement of the problem offers a means to describe propagation of localized shear bands, this being its advantage over the classical approach. Fig. 2 shows the calculation by different models compared with the experiment.

LBP at the mesolevel is responsible for the appearance of a yield tooth and a yield plateau on the macro stress–strain curves. Let us consider this in greater details. In Fig. 3 we can see a part of the stress–strain curve calculated for the strain rate of 50 \( s^{-1} \). In the calculation, we prescribe for the plastic shears to be originated near boundary \( BC_1 \) by using for this region only one rule given by Eq. (8) to describe the yield criterion. Local regions near the surface begin to plastically deform, provided the effective stress (10) reaches its critical value defined by the strain hardening law \( f(\varepsilon_{\text{eff}}^p) \).

All components of the deviator stress tensor in these local regions relax in accordance with the law of relaxation, which results in a time dependent accumulation of plastic strains. Other regions continue to deform elastically because the criterion of plasticity covers both Eqs. (10) and (11). Then effective plastic strains in the regions near \( BC_1 \) reach the critical value \( \varepsilon^* \), and another region close to this region is involved into plastic deformation. Thus, plastic deformation propagates along direction \( x_1 \) in a step-by-step mode. Plastic strain patterns for different moments (a)–(d) of the shear band propagation are presented in Fig. 4. Boxes in Fig. 3 mark the respective macro stress–strain behavior. At the first steps of the process, the value of plastic strain in a small region near surface \( BC_1 \) is not enough to relax stresses throughout the re-
region under study. As a result, we can see a yield tooth on the stress–strain curve. As the shear band propagates away from surface $BC_1$ there occurs stress relaxation that results in a descending portion on the average stress–strain curve (Fig. 3, box a). The relaxation comes to an end when the plastic deformation covers approximately a half of the calculation region (Fig. 4(b)), which reduces the average stress. This corresponds to the lower yield point on the stress–strain curve (Fig. 3, box b). Then strain hardening in the plastically deformed region (Fig. 4(c)) begins to influence macro response (Fig. 3, box c). Finally, the plastic strain front arrives at the opposite end (Fig. 4(d)), all the region $A(x,t)$ is plasticity deformed, and mesophenomena no longer influence the macro stress–strain behavior (Fig. 3, box d).

We introduce strain rate sensitivity into the model formulation as well. The first run of calculations was made using relation (14) to describe relaxation properties of the steel. Fig. 5 shows the calculated stress–strain curves for different strain rates in comparison with the experimental data. The following values of the parameters were chosen to fit the experimental dynamic properties of the material within the range of strain rates from quasistatic loading to $10^2$ s$^{-1}$: $A = 1.1 \times 10^{-4}$ s; and $B = 3$ MPa s. For the strain hardening function, we derive an expression of the type

$$f(e_{\text{eff}}^p) = 5.13 + 4.2e_{\text{eff}}^p - 219.2 \cdot e_{\text{eff}}^{2p},$$

where the numerical coefficients have GPa-dimension.

Quadratic dependence (18) allows us to adequately describe a real shape of the stress–strain curves in a wide range of strains up to 10% and higher. From Fig. 5, we can see a good agreement between calculated and experimental data. Macro behavior is most precisely described for both the quasistatic stress–strain curve and the stress–strain curve at the highest strain rate of $10^2$ s$^{-1}$. The difference between calculations and experiment for the curves lies within the range of 0–2.5%. The maximum difference of $\approx 10\%$ is seen for the strain rate of 10 s$^{-1}$. It should be noted that the lower the range of strain rates to be simulated using Eq. (14), the better the agreement with the experiment. And vice versa, if we obtained parameters in (14) for a wider strain rate range than the above-mentioned, there would be a higher maximum difference between calculated and experimental data.

To describe the stress–strain curves for high macro strain rates, we suggest to use another dependence for the relaxation factor. This relation prescribes for $\eta$ to be a function of time in an explicit form (Eq. 15). In this case, for the material

Fig. 4. Stress and plastic strain patterns for different times shown by squares in Fig. 3.

Fig. 5. Stress–strain curves for the 20MnMoNi55 steel at different strain rates calculated using Eq. (14). Experiment [10].
investigated the model constants are of the following values: \( A' = 2.7 \times 10^{-3} \text{ s} \); and \( B' = 1.3 \text{ GPa} \). The use of this simple equation allows us to match experimental and calculated macro behavior within the strain rate range of \( 10^2 –10^3 \text{ s}^{-1} \). The respective results of numerical simulation are presented in Fig. 6. It is clear from the figure that the difference between calculation and experiment does not exceed 5% within the strain range investigated. The yielding function in Eq. (13) was assumed to be constant: \( f = \text{const} = 530 \text{ MPa} \). For the steel in question, this value is the experimental yield point under quasistatic loading. Thus, in this case there is no quasistatic strain hardening in the model formulation, and step-by-step increase in averaged macro stress on the stress–strain curves is achieved via a dynamic balance between the external stress applied and material relaxation response only. We should note the fact that this formulation includes three model constants instead of five, while describing the process using the quasistatic strain hardening function (Eq. 18).

We should mention that all differences between calculation and experiment were estimated within the strain range except for the LBP region (Fig. 5). This is due to the following reasons. A large number of experimental investigations show that before the experiment we do not know exactly the region of the testpiece, where a Luders band front initially originates. In one test, the band originates near one grip of the testing machine, in another test—near the other, in the third test plastic deformation propagates from both ends of the testpiece in opposite directions. As a result, macro stress–strain behavior for a certain type of material in the LBP region may vary from one test to another. According to physical mesomechanics, the problem of plastic shear generation can be treated in terms of local stress concentrations near the interfaces, but this issue needs additional investigation, which is beyond the scope of this paper. There is one more reason for this estimation of the difference. Experimental techniques use electronic gauges to measure relative elongation. The gauge location and arrangement on the working part of the testpiece may be slightly different, so they would measure different macro strains. For uniform deformation, this fact is not so critical. However, considering LBP, which is a strongly non-uniform process, we have to take this fact into account. To investigate this problem numerically we carry out the following calculations. Fig. 7 shows the stress–strain curves for different strain measurements. Bold solid line corresponds to the stress–strain curve for the strain rate of 100 \text{s}^{-1} presented in Fig. 5, where we measure relative elongation of the whole region \( A(x,t) \) in direction \( x_1 \). Using symmetry boundary conditions (Eq. (17) for \( BC_3 \)), we prescribe for the Luders band to propagate from both ends of the testpiece. Curves \( a \) and \( b \) reflect macro behavior in the case of measuring strain for the regions (a) and (b) in Fig. 1, respectively. And curve \( c \) corresponds to the case of LBP only from one end of the testpiece.

![Fig. 6. Stress–strain curves for the 20MnMoNi55 steel at different strain rates calculated using Eq. (15). Experiment [10].](image1)

![Fig. 7. Calculated stress–strain curves for different strain measurements.](image2)
Stress for all cases was measured according to Eq. (18) for the whole region $A(x,t)$. We can see from the figure that the results calculated differ from one another.

The value of the model parameter $e^*$ is responsible for certain values of the upper and lower yield points, as well as for the value of the LBP strain on the stress–strain curves (Fig. 5). But in view of the above discussion it is not enough for us only experimental macro stress–strain curves to obtain real value of this constant reflecting material property at the mesoscale. We need here additional experimental evidence: for the certain experimental stress–strain curve it is necessary to know exactly the place, where the Luders band originated. We selected the value of $e^* = 0.4\%$ to agree the calculations with experimental stress–strain curves, suggesting for Luders band to originate near the grips ($BC_1$ in Fig. 1).

To correctly obtain physical value of $e^*$ for a certain material, we need the experimental data on both macro stress–strain behavior and micro–mesostructure during the loading or/and to introduce plastic shear generation from first principles into the model formulation.

4. Conclusion remarks

To sum up, the results obtained lead us to conclude that

- mesoscale LBP can be simulated introducing into the model the methods of both continuum mechanics and discrete cellular automata. This combined formulation makes it possible to calculate the appearance of the yield tooth and the Luders plateau on the stress–strain curves as well as to investigate numerically the non-uniform stress–strain state while plastic front propagates through the testpiece;
- the use of both a linear time dependent relation for the relaxation factor and a quadratic strain hardening function allows us to arrive at an agreement between calculated and experimental stress–strain curves in a wide rage of strains and strain rates.

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