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MICROSTRUCTURE-BASED NUMERICAL MODELLING OF MANUFACTURING PROCESSES OF NANOLAYERED MATERIALS

Recent development in the field of numerical modelling of innovative manufacturing processes, in which nanolayered materials can be produced, is presented in the paper. Combination of the Angular Accumulative Drawing, continuous wire drawing and wire flattening were used to produce thin nanolayers that will be used for subsequent production of nanolayered metal strips using Accumulative Roll Bonding process. Proposed methodology combines microstructural aspects of deformation such as strain-induced precipitation processes and development of dislocation substructures. Additionally, multiscale modelling approach based on the 3D Digital Materials Representation was utilized to support experimental research and to investigate inhomogeneous material behaviour during deformation. Proposed methodology provides a possibility of forming materials, which are e.g. difficult to form in a conventional manner. Advantages and limitations of the proposed model are summarized and discussed with respect to its potential application to precipitation strengthened bcc nanolayered materials.

1. INTRODUCTION

Rapid development in various branches of the industry that use steel products (constructional, automotive, aerospace, military etc.) brings along new requirements that have to be met by the metallic materials that are used in these fields of applications. Higher strength, better impact energy absorption, toughness and crack initiation resistance are the examples of the properties that enhancement is still expected. One of the most effective ways to improve the properties is grain refinement. For the last two decades there has been a lot of progress made in the field of production of ultrafine-grained (UFG) and nanostructured structures in various metals and alloys including steels [1]. Two main routes that use “top down” manufacturing approach can be distinguished i.e. Severe Plastic Deformation (SPD) and Advanced Thermomechanical Processing (ATP) [2]. The first one

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utilises high accumulation of deformation energy to refine the microstructure down to submicron level, while the second one controls microstructural phenomena at hot and warm deformation regime such as static and dynamic recrystallization, strain-induced precipitation process or strain-induced dynamic phase transformations.

High strength in UFG materials is usually achieved at the expense of the ductility due to limited uniform elongation resulted from the lack of work hardening. One of the solutions to overcome this problem is to produce a bimodal or gradient microstructure, where bimodal grains will be responsible for good strength while coarse grains will provide work hardening, and thus, will keep a required level of ductility. Another way of improvement of ductility in UFG and nanostructured steels is a use of the strengthening effects of solid solution and second phase particles. This strengthening mechanism is characteristic for microalloyed steels where a large volume fraction and a fine dispersion of a second phase effectively increase the work hardening rate by promoting the accumulation of dislocation around interphase boundaries and delay the strain localisation. Extensive research in the area of proposing a strong and yet ductile UFG or nanomaterial that may be produced in the continuous manner resulted in a new group of the products where the microstructural features are organised in clusters or layers. These materials may be produced using a combination of SPD and ATP methods. For example, recently developed Accumulative Angular Drawing (AAD) [3],[4],[5] combined with wire drawing (WD) and wire flattening (WF) processes may be employed and effectively used to induce SPD effects in microalloyed steel wires. The AAD is characterised by a complex strain path history resulting from various deformation modes. Its main purpose is to produce wires that represent increased strength and ductility due to controlled deformation inhomogeneity [2].

With a more complex strain path and more energy accumulated in the wires during the AAD process one should expect stronger microstructural effects and mechanical property changes in the drawn wires compared to the conventional wire drawing process [2],[6]. However, despite the considerable progress, no clear methodology exists for transferring this information into a predictive macroscopic description of produced in such way materials. It has been already found that thanks to the numerical modelling tools, better control of the processes parameters during AAD [7] it is possible to introduce controlled inhomogeneity of strain and, by accumulation of the deformation energy, to induce grain refinement across the cross-section of the wire. Combination of complex metal forming processing (ADD and successive flattening and accumulative roll bonding) leads directly to typical for the SPD techniques microstructural effects, i.e. formation of ultrafine-grained and finally multi-layered structural material. It is well known that such materials represent a unique laminated or layered composite form that thanks to exceptionally attractive combination of mechanical properties allows them to exceed the limits that exist in even the most advanced structural materials [8]. Therefore, the main objective of the present work is a development of the numerical tool that will allow better understanding of the deformation effects occurring during described metal forming processes. Because of the complexity of the deformation mechanisms and high microstructural inhomogeneity of produced nanolayered materials, the microstructure-based modelling approach has to be undertaken. Fundamentally different deformation mechanisms that control the mechanical behaviour of nanolayered materials, result from complex processing routes and fine scale features

present in the microstructure. Its proper representation in the computer simulation requires then multiscale modelling approach with properly defined materials models. It is expected in the present study, that changes in the mechanical response of precipitation strengthened nanolayered materials are closely related to the movement of dislocations in a flattened grains, what is changed significantly by the reversal of stress during applied complex deformation processing. Therefore, in the present work, various modelling approaches will be proposed and discussed with respect to their applicability in the modelling of nanolayered materials.

2. EXPERIMENTAL SETUP

In order to assess the interrelationships between processing-microstructure-mechanical behaviours of UFG layered microstructure, microalloyed steel wire rod ($\Phi 6.5\text{mm}$) with a basic chemical composition being (in wt. %) 0.07C/0.29Si/1.36Mn/0.067Nb/0.03Ti/0.0098N/0.003B was used in the current work. The initial microstructure, presented in Fig. 1, consisted of uniform and quasi-polygonal grain structure with a mean grain size of $12\mu\text{m}$. Due to the complex effects of various strengthening mechanisms present in microalloyed steel, this constructional material is widely used, and thus, it is very interesting from the research perspective.

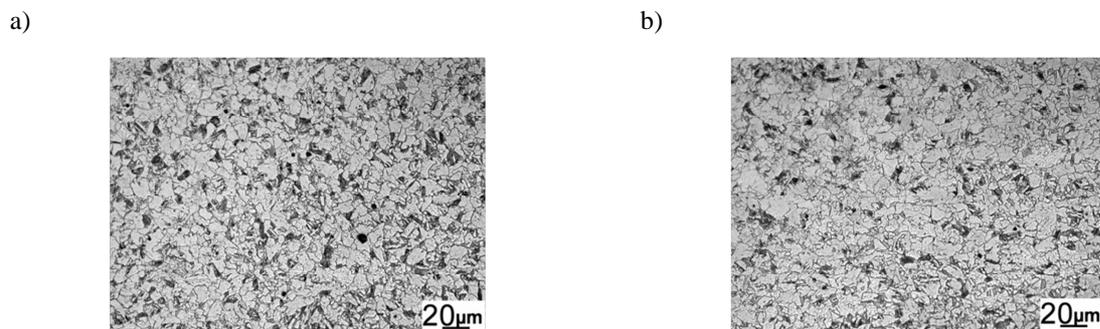


Fig. 1. The initial microstructures of the studied material taken in from: a) longitudinal and b) transverse cross-section of the supplied wire rod

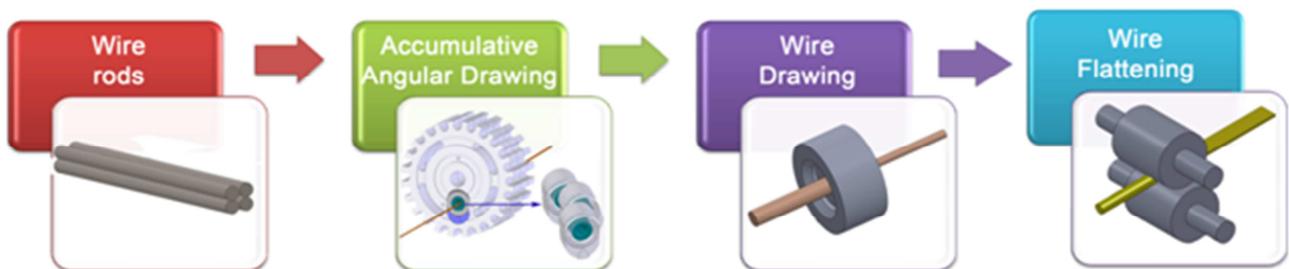
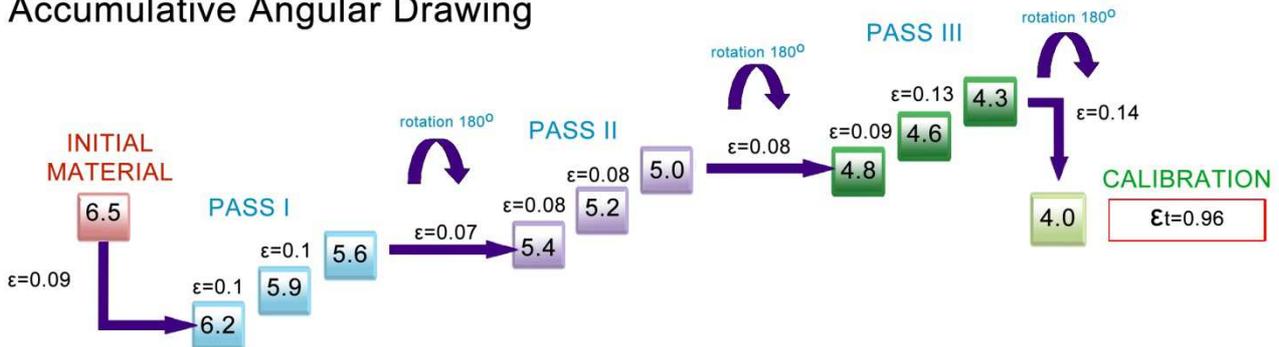


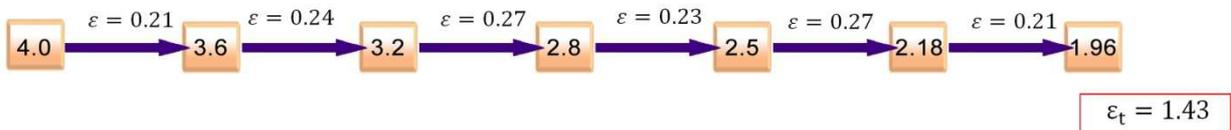
Fig. 2. General sequence of the deformation processes used in the current work to produce UFG layered material

The production process of UFG layered material was carried out according to the general sequence presented in Fig. 2. First, AAD process was performed to introduce severely deformed and inhomogeneous microstructures in the drawn wires. In this process, three deformation passes were applied (according to Fig. 3) and final wire diameter after AAD was 4.0mm. Next, a multi-pass linear wire drawing (WD) process was carried out until wire diameter was reduced down to 1.96mm. Finally, produced in such way wires were additionally deformed by wire flattening (WF) with equivalent strain of 0.45 to the thickness of 400 μ m, so that the total strain accumulated in all processes was $\epsilon = 2.81$ (see: Fig. 3).

Accumulative Angular Drawing



Wire drawing



Wire flattening



Total strain $\epsilon_t = 2.85$

Fig. 3. The experiments scheme presenting the deformation schedule of the combined SPD processing

The general sequence of the research performed in the present work was as follows: first, preliminary study on the assessment of the initial material and design of the deformation schedules of the combined SPD processing was performed. Then, microstructural analysis of the obtained microstructures was carried out using optical, transmission electron microscopy (TEM), scanning electron microscopy (SEM), and electron backscatter diffraction - EBSD). At this stage mechanical properties of obtained UFG layered materials were also assessed using tensile and hardness testing. Finally, all the data gathered during all the above-mentioned stages were extracted for further computer modelling purposes.

3. RESULTS

In the present work, the most characteristic microstructural features that were identified in the obtained materials are fine grains, subgrains, dislocations and fine precipitates. Examples of the microstructures that were obtained after combination of AAD, CWD and WF are summarised in Fig. 4. Both from the EBSD maps (Fig. 4a, b) and TEM bright field image (Fig. 4d) it can be seen that in the severely deformed specimens the initial grains are elongated - especially in the area close to the surface region.

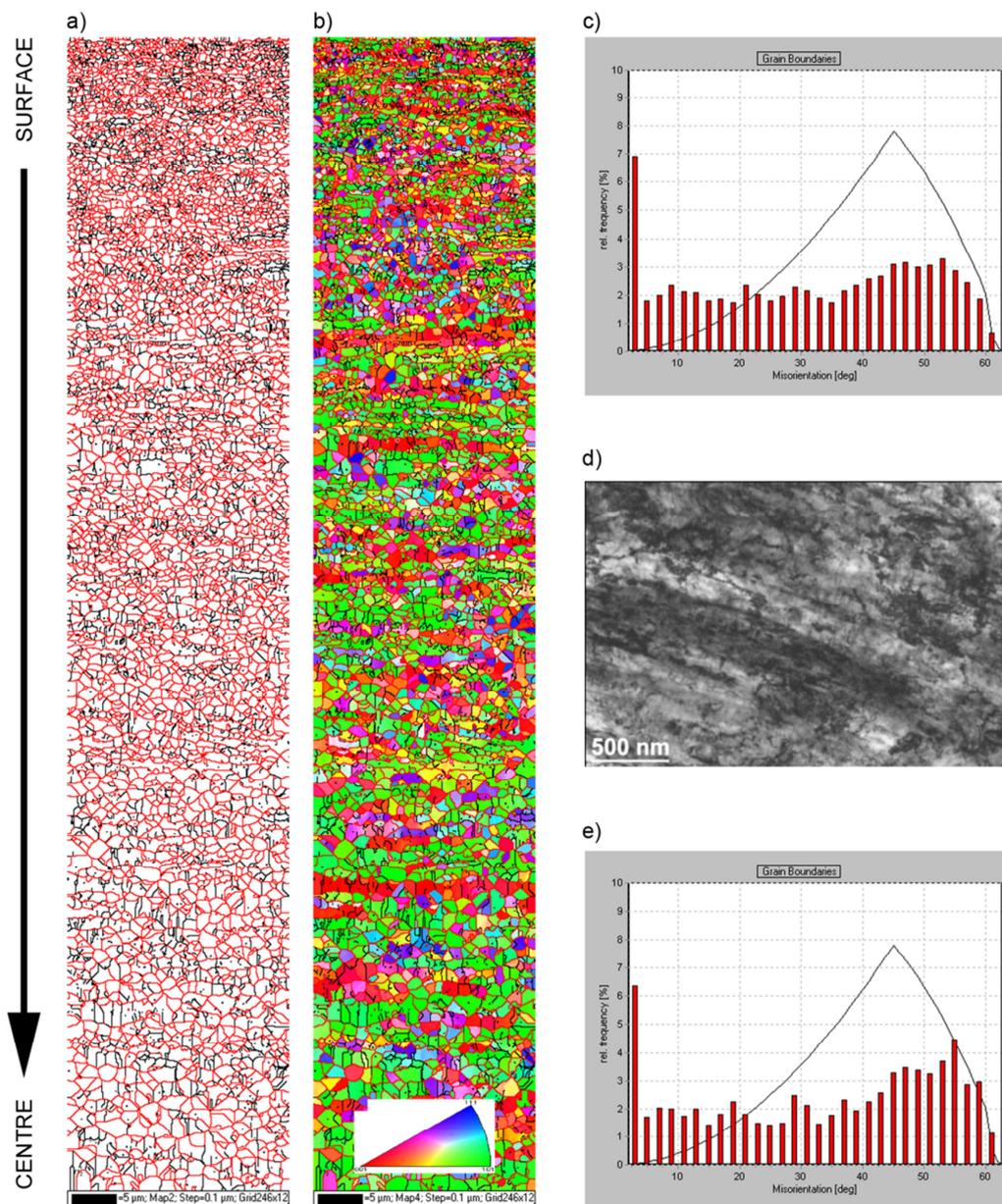


Fig. 4. EBSD results showing maps of a) grain boundaries and b) crystallographic texture at the cross section of the studied material obtained after AAD, CWD and WF. c,e) grain boundaries distribution histograms taken in the areas close to the surface and the centre of deformed material d) TEM bright field image of the deformed specimen

Additionally, it can be noticed that the misorientation angle distributions are similar across the sample thickness, however, the spacing between high angle grain boundaries decreases significantly as one moves towards the surface leading to inhomogeneous lamellar submicron structure yet characterised by high number of dislocation boundaries and disperse precipitates (Fig. 4d). Another noticeable phenomenon observed in severely deformed wire specimens is the refinement of the pearlite colonies what, as should be expected, directly leads to increased ductility and decreased strength of the investigated material. However, in the present study the strength loss is effectively limited thanks to the presence of other sources of strengthening that operate in the UFG microalloyed steels i.e. precipitation, solid solution strengthening mechanisms as well as grain refinement (Hall-Petch strengthening) – Fig. 5.

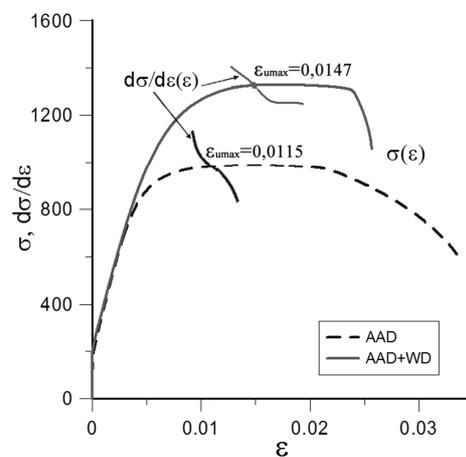


Fig. 5. Stress-strain curves obtained under quasi-static tension tests of the specimens after AAD and AAD+CWD processes with marked uniform elongation values assessed using Considère criterion

Additionally, Considère criterion was utilised to assess the ductility of obtained UFG wires. Uniform plastic deformation occurs as long as the true stress is below the value of the work-hardening rate ($d\sigma/d\varepsilon < \sigma$). Maximum values of uniform elongation connected with the onset of necking during the tensile test are shown in Fig. 5. It can be noticed that not only enhanced strength, what was expected when total equivalent strain increases, but first of all increased ductility was obtained in the wires produced after combined AAD+WD comparing to the specimens treated only with the AAD process. It is believed that the presence of fine precipitates and refined pearlite colonies were the two main factors contributing to the improvement of the strength to ductility ratio in the obtained wires.

4. MICROSTRUCTURE-BASED MODELLING

The aim of the second part of the work was to build a numerical model of the above-described manufacturing processes in order to study the effect of the applied processing

parameters on the deformation behaviour and inhomogeneity of the produced nanolayers. In order to take into account microstructural features in an explicit manner, Finite Element (FE) multiscale modelling approach based on the 3D Digital Materials Representation (DMR) [9] was utilised.

Due to the fact, that analysed processes are highly nonlinear, i.e. material during deformation undergoes multiple strain reversals, there was a need to use a properly defined material model, that takes into account strain path changes. Therefore, the first step to establish a properly defined robust computer model, was an analysis of existing constitutive material models with respect to their accuracy in the prediction of flow behaviour of materials subjected to complex deformation modes. In order to do so, cyclic torsion test was carried out using cylindrical test specimens (with gauge diameter of 10mm and gauge length of 20mm) that were made from S460M steel with basic chemical composition 0,13C/0,49Si/1,49Mn/0,035Nb/0,003Ti/0,006N. The experiment was conducted at room temperature. Standard cylindrical torsion specimen with the strain gauge diameter of 10mm and gauge length of 20mm was deformed in a cyclic manner applying forward / reverse torsion with the strain of 0.25 per pass and the strain rate of $0,1s^{-1}$. During the test, twist angle and torque were recorded and subsequently converted into equivalent plastic strain vs equivalent plastic strain curves using standard equations. Then, numerical model of this cyclic forward/reverse torsion test was developed using Abaqus Standard.

Subsequently, three existing constitutive models were chosen from the literature and implemented to the numerical simulation of the torsion tests.

First selected model was Chaboche model [10]. It consists of isotropic and kinematic hardening components. The first one can be described by the following equation:

$$\sigma^0 = \sigma_0 + Q(1 - \exp^{-b\varepsilon}) \quad (1)$$

where: σ^0 – isotropic part of hardening; σ_0 – yield stress; Q – maximum change in yield surface, b – rate of change of yield surface during plastic deformation; ε – strain.

Evolution law of the kinematic part of the Chaboche hardening model is described as a sum of the backstresses, which includes parameters that control the position of the stress for each backstress:

$$\dot{\alpha} = \frac{C_k}{\sigma^0}(\sigma - \alpha)\varepsilon - \gamma_k \alpha \varepsilon \quad (2)$$

where: C_k – initial kinematic hardening modulus; γ_k – the rate at which the kinematic hardening modulus decreases with increasing plastic deformation; σ^0 – the size of the yield surface; σ – stress tensor; α – backstress; ε – plastic strain.

This model is widely available in various finite element simulation packages and it can be effectively used in simulations where the strain path changes take place.

The second chosen model was Johnson-Cook model [11]. It is a phenomenological model, i.e. it is based on traditional plastic theory that reproduces several important material responses observed in impact and penetration of metals. The three key material responses are strain hardening, strain-rate effects and thermal softening. These three effects are combined in this model in a multiplicative manner:

$$\sigma_y = [A + B(\varepsilon_{ef}^p)^n](1 + C \ln \dot{\varepsilon})(1 - (T_H)^m) \quad (3)$$

where: ε_{ef}^p – effective plastic strain, $\dot{\varepsilon} = \frac{\varepsilon_{ef}^p}{\varepsilon_0}$ – where ε_0 strain rate used to determine A, B and n, $T_H = (T - T_r)/(T_m - T_r)$ where T_m melt temperature, T_r reference temperature when determining A, B and n.

Due to the fact, that in microalloyed steels the presence of the precipitation and solid solution strengthening mechanisms significantly affects the hardening process, mostly due to the retardation of dislocation substructure formation process, the third analysed rheological model was dislocation-based hardening model that was proposed in [12]. In the dislocation density work hardening model, because a significant rearrangement of the dislocation substructure occurs during strain reversal, dislocation density as a model parameter is introduced. In this model the dislocation density is separated into two components that are associated with the forward and reverse loading/unloading of the dislocation substructure. General formula for the stress of the considered model is based on the Kocks model and can be shown as follows:

$$\sigma = \sigma_0 + M[X + (1 - \alpha)(\tau - \tau_0)] \quad (4)$$

where: σ_0 – is the initial stress, M – is the Taylor factor; τ_0 – is the stress related to lattice friction and solute contents. Concerning the backstresses, an internal variable X is introduced to describe the rapid changes in stress under reverse deformation:

$$\dot{X} = C_x(X_s \dot{\gamma} - X|\dot{\gamma}|) \quad (5)$$

where: C_x – is a constant that characterises the dynamics of the back stress changes, $X_s = a(\tau - \tau_0)$, (a – fraction of the stress that experiences some delay in development of the backstress). Shear stress can be calculated from:

$$\tau = \tau_0 + \alpha G b \sqrt{\rho_f + \rho_r} \quad (6)$$

where: G – is the shear modulus, b – length of the Burgers vector and α – a factor that weights the dislocation interaction. Dislocation density parameter consists of two components that are related with forward and reverse loading of dislocation substructures:

$$\frac{d\rho_f}{d\varepsilon} = \frac{1}{b\lambda} - f\rho_f \quad (7a)$$

$$\frac{d\rho_r}{d\varepsilon} = \frac{1}{b\lambda} \cdot \frac{\rho_r}{\dot{\rho}_f} \quad (7b)$$

$$\rho_f(\gamma_f = 0) = (1 - p)\dot{\rho}_f \quad (8a)$$

$$\rho_r(\gamma_f = 0) = p\dot{\rho}_f \quad (8b)$$

where: the athermal storage that depends on the mean free path Λ for mobile dislocations – Eqs. 7a and 8a, and the thermally activated recovery term whose efficiency is given by the factor f that depends on the temperature and strain rate – Eqs. 7b and 8b.

The model coefficients, in the case of Johnson-Cook model, were taken from the literature for HSLA steels, whereas in the case of Chaboche and work-hardening models they were calibrated using inverse approach and can be found in [13].

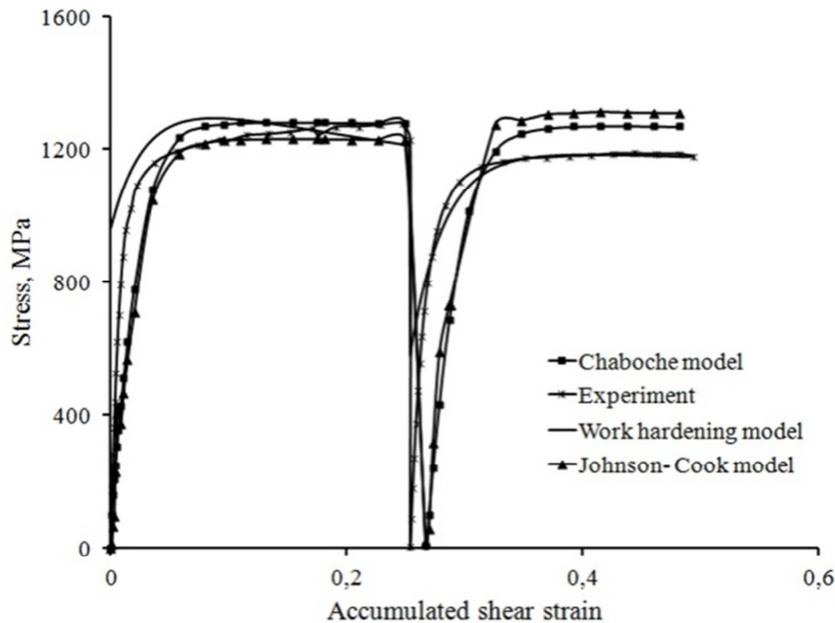


Fig. 6. Comparison of the measured and calculated flow stresses using tested models

Comparison of the calculated and measured flow stress for all tested models is presented in Figure 6. It can be seen that the best prediction was achieved using dislocation density work hardening model whereas the least accurate results were obtained using Johnson-Cook model. It is due to the fact that this model is based on the isotropic hardening only i.e. does not take into account effects of strain path sensitivity (such as Bauschinger effect and so on). Therefore, the application of the combined hardening models such as Chaboche model is strongly recommended for the simulation of nonlinear deformation processes and this model was selected for further work.

The general idea of the multiscale model of analysed processes of manufacturing of nanolayered materials is presented in Fig. 7. Submodelling technique was used as an efficient tool to bridge the scales. In this approach, a global model with coarse FE mesh is run first and then, based on the displacements of the nodes, a local model with a much finer mesh is run in a local domain. This is an effective way to get a detailed numerical solution at fine scale in the case when a global simulation would require very large number of elements.

In the present work, due to the complexity of the whole deformation process, a concurrent multiscale approach based on two steps of submodelling was proposed. First,

global models of AAD, CWD and WF processes were simulated in Abaqus Explicit using eight-node hexagonal reduced integration elements and hourglass control (C3D8R) – Fig. 7. AAD, Drawing of 2000mm long wire with an initial diameter of 6.5mm through the set of three AAD dies and six linear dies down diameter of 1.93mm was simulated first. Then simulation of wire flattening to 400 μ m strip was performed.

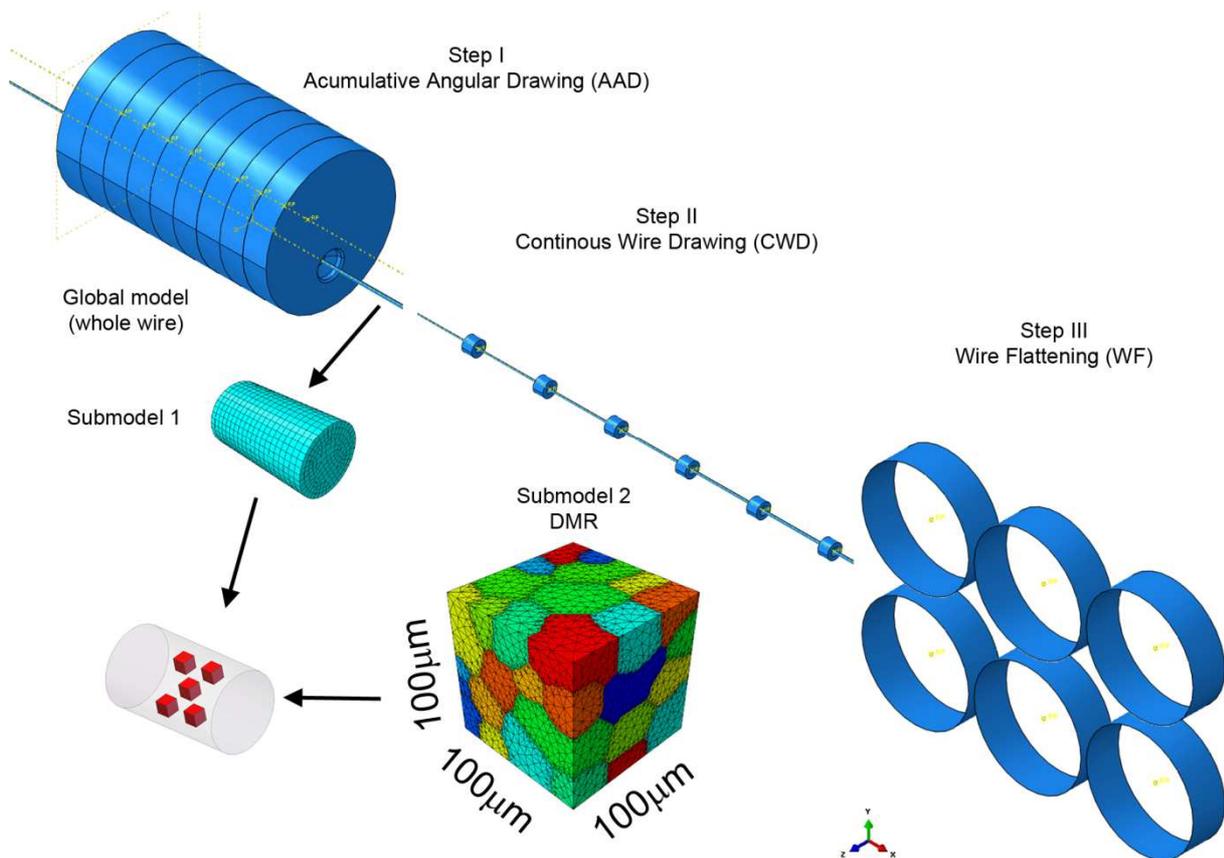


Fig. 7. Multiscale computer model of the nanolayered steel's manufacturing process

Furthermore, the analysis was repeated on a smaller cylindrical area (10mm long) extracted from the global model using Abaqus Standard, and a much finer mesh was used (see: Fig. 7). Finally, a second submodel was generated using the Digital Materials Representation approach (DMR) [9], and calculations were performed again using Abaqus Standard – Fig. 7. A set of 5 volumetric unit cells ($100\mu\text{m}^3$) was created in order to capture the effect of the process on strain inhomogeneity. Additional emphasis was put on the proper representation of the effects of precipitation hardening that are characteristic for investigated here microalloyed steels. The idea of taking into account this strengthening mechanism is presented in Fig. 8. DMR unit cell was created as a two phase material i.e. steel matrix with dispersed fine particles of the Nb(C,N) precipitates. The properties of the steel matrix were assigned to each grain separately using material data generated from Chaboche model (slightly diversified according to Gauss function in order to take into

account crystallographic orientation changes of the grains). The size of the Nb(C,N) particles was chosen based on the graph presented in Fig. 8. Precipitation strengthening is a hardening mechanisms that can be governed by two mechanisms - depending on the type and size of the particles [14]. In the first mechanism, dislocations moving during deformation can cut through the particles that are larger, softer and yet coherent with the matrix - Mott-Nabarro mechanism. Finer and harder particles (e.g. strain-induced precipitates of Nb(C,N)) that cannot be cut through moving dislocations work as obstacles for them so they can only be by-passed what causes much higher strengthening effect - Orowan mechanism. As it can be seen from Fig. 8 there is an optimal size of the second phase particles that causes maximum strengthening effect - for Nb(C,N) it is around 10-50nm. In the present work, hard particles with this size range were created within the DMR unit cells.

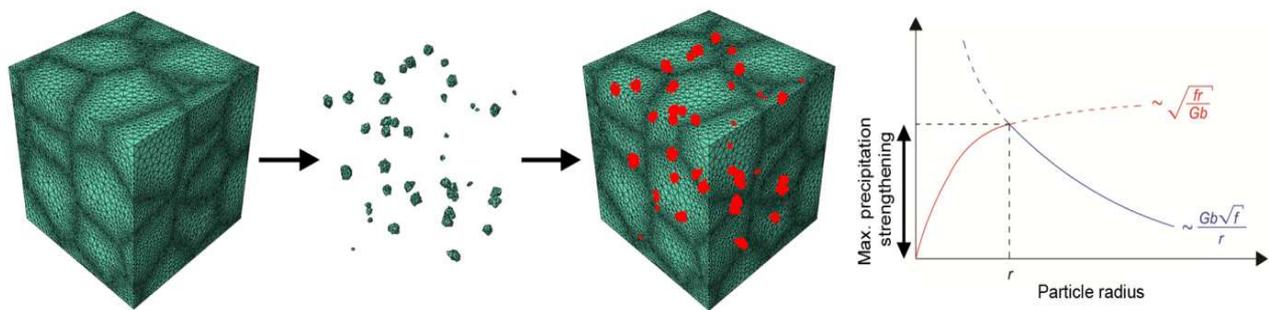


Fig. 8. Way of taking into account the precipitation hardening effects in the current modelling work

5. INITIAL MODELLING RESULTS

As mentioned earlier, the main aim of the present work is a development of the multiscale model of AAD, CWD and WF in order to optimise production of the nanolayered materials. At the current stage, global models of all considered processes were developed. Simulations using DMR approach at local scale are still under development - at the moment only simulation of AAD process has been finalised. Examples of calculations after 1st and 3rd pass of AAD process are presented in Fig. 9 and 10 respectively. Distribution of Mises stress in the global model and at two key positions of the transversal cross section of the drawn wire after the first pass of drawing through the 3rd die of AAD is presented in Figure 9. It can be seen, that thanks to the application of the multiscale approach, much more details concerning stress distribution at various positions of the drawn wire can be obtained. This approach seems to be very promising, as representation of the microstructural features at various scales, offers much more physically-based numerical tool for the simulation of the processes characterised by a complex strain path history.

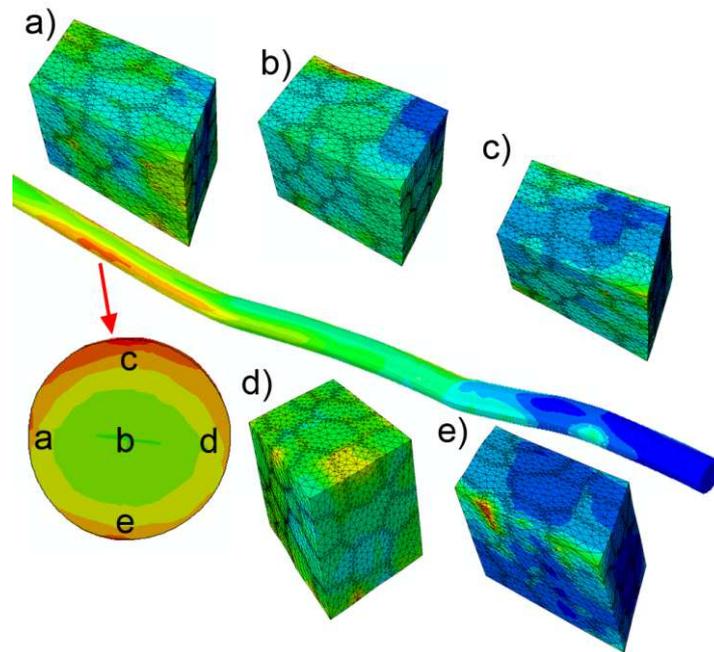


Fig. 9. Examples of calculations. Equivalent plastic strain in drawn wire after 1st pass of AAD drawing. Global model and unit cells attached at various positions of the wire's cross-section (indicated by letters a - e)

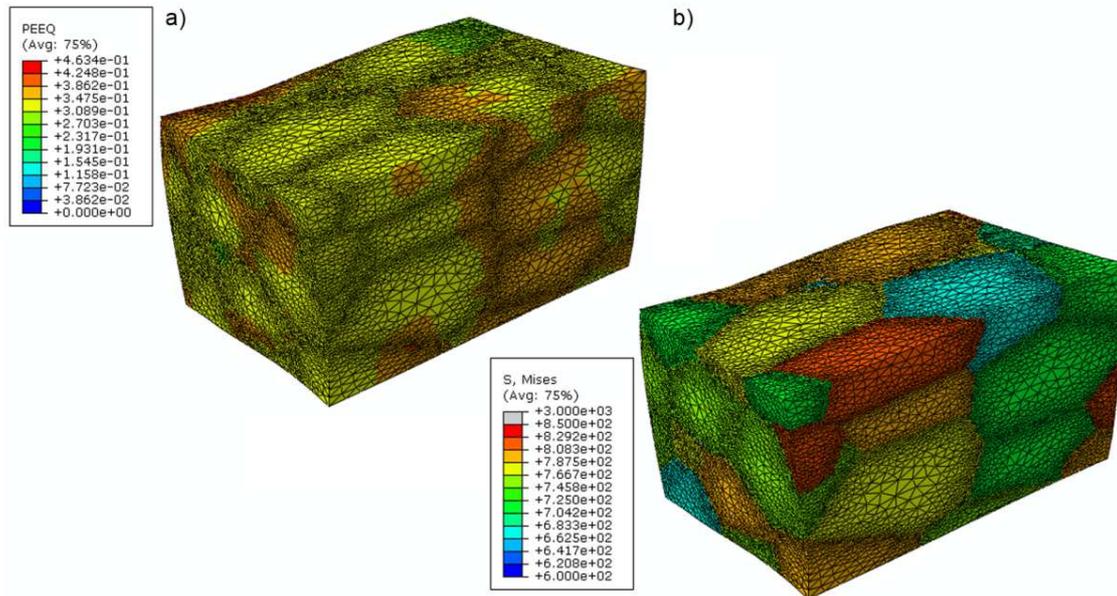


Fig. 10. Equivalent strain -a) and equivalent Mises stress -b) distributions in the DMR calculated in the centre of the cross section of the wire after 3rd pass of AAD drawing in the 3rd die

Figure 11 shows initial modelling results of the wire flattening process using global model. It can be seen that the model properly captures the effects of complex deformation

history and shows potential in the prediction of the material deformation behaviour in this process. However, at the current stage it is not possible to properly assess it in the more detailed way as there is a need to obtain the results at local scales from the preceding processes (AAD +CWD) what will be the next step of the work.

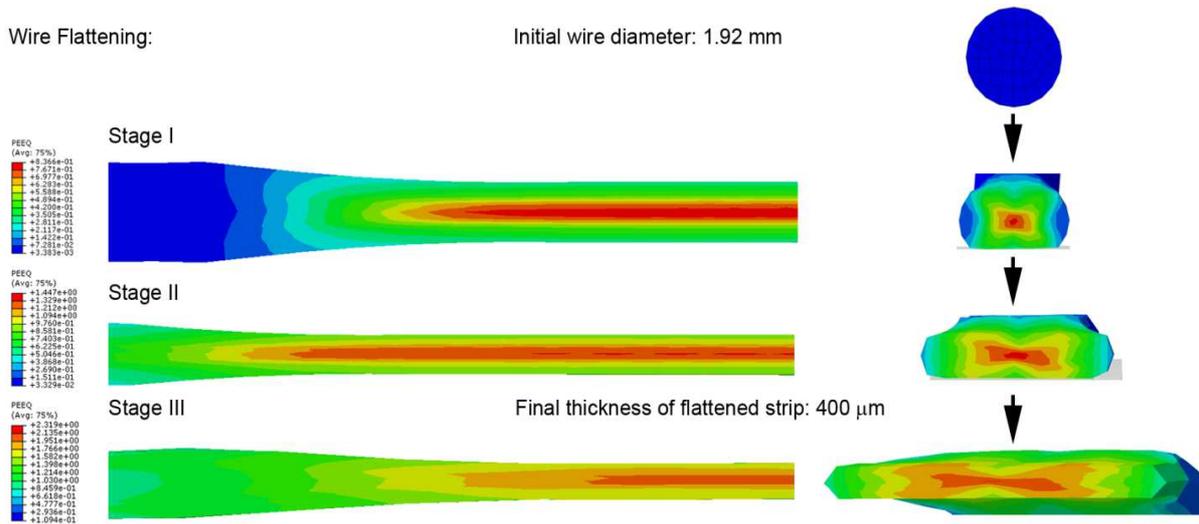


Fig. 11. Equivalent plastic strain distributions calculated in global models of wire flattening process

6. CONCLUSIONS

In the present work, studies of the development of nanolayered structure in microalloyed steel was performed. Manufacturing process including angular accumulative wire drawing, followed by continuous wire drawing and wire flattening processes (i.e. “top-down” systems of the grains refinement process) was proposed. In the second part of the work, numerical model of these processes was developed and used to study the effect of processing parameters on the deformation behaviour of produced materials. It was shown that multilayered ultrafine-grained microstructure can be effectively produced using proposed methodology. Initial modelling results show the potential of the applied microstructure-based multiscale modelling strategy. Utilisation of the strain path sensitive constitutive model in the multiscale analysis is crucial in order to effectively model the complex strain path processes and to control strain and microstructure evolution, and thus, to optimise the properties of the final products.

ACKNOWLEDGEMENTS

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