Effects of modified surface layer and grain size on surface roughening in steel specimens

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Abstract

This work is concerned with the numerical analysis of modified surface layer and grain size influence on surface roughening in a high-strength steel under uniaxial tension. Using a three-dimensional finite-difference model, numerical simulations are conducted. The study suggests that the modified surface layer exercises significant influence over the origin of strain heterogeneity. The results show that height of ridges grows and surface roughness develops with increasing average grain size. Also it is supposed that more grains affect surface roughening in the fine-grained material comparably to coarse-grained one.

1 Introduction

From the mesomechanical viewpoint the surface layer of a solid under loading is a specific structural level which plays an important role in the deformation response of the material [1],[2]. Plastic deformation of polycrystalline metals is known to induce surface roughness [2] which is undesirable phenomenon for many applications in industrial practice because it deteriorates surface reflectivity, weldability and mechanical characteristics of the material due to plastic strain localization. On the other hand, according to the approach of physical mesomechanics, all deformation defects originate in the surface layers of solids [1],[2]. Hence, the surface changes may be an indicator of the material internal state and can be used in the field of nondestructive control. Thus, in order to develop effective methods to take surface roughening under control we have to understand this phenomenon. Despite a great deal of pertinent experimental and numerical evidence, the mechanisms involved and the factors responsible for the resulting roughening patterns is yet a debated topic among researchers. This is of particular importance to investigate deformation processes at the meso level. It is particular significant that not individual grains but their larger sets are involved in cooperative motion to form folds, hills and hollows.

Previously [3],[4] we investigated experimentally and numerically the details of surface roughening in steel specimens under uniaxial tension. We analyzed the high-strength steel EK-181 [5] that is used for fast breeder reactor rod claddings. With the using of rupture atomic force microscope surface roughening phenomena was investigated at the mesoscale in situ in uniaxial tension. In a model we developed to perform a numerical investigation, the structural heterogeneity was taken into account explicitly through the dependence of physical-mechanical properties (density, yield strength, etc.) on the coordinates. The three-dimensional model of a polycrystalline structure was generated by a step-by-step packing method [6] on a regular grid. Mesoscale surface roughening was studied with the aid of a three-dimensional finite-difference model. The general mechanisms of this phenomenon in plastically deformed steel were shown. The results obtained suggest that the internal interfacial inhomogeneities are responsible for the formation of the surface roughness on the examined free surface. A clearer understanding of the stress-strain state responsible for the out-of-plane displacements on the free surface of three-dimensional polycrystals with a periodic structure was gained.

In this work the effects of two different factors known to influence surface roughening such as modified surface layer and grain size are analyzed numerically. The formation and evolution of a deformation-induced relief in polycrystalline materials with different grain size with and without modified surface layers were studied in the context of physical mesomechanics. The three-dimensional finite-difference model proposed in [4] was modified to investigate the roughening behavior of high-strength steel with nanostructurized surface layers and with different grain size in the bulk.

2 Microstructure-based model

Problem of the uniaxial tension of polycrystalline structures with and without modified surface layer as well as those with different grain sizes in the bulk of the material was examined in a three-dimensional statement. In order to describe the dynamic deformation of polycrystals a system of equations including the balance laws of mass, momentum, kinematic relations and constitutive equations was numerically solved. The detailed formulation of the problem can be found elsewhere [6]. So let us start by a briefly describing the constitutive model.

In the roughening simulations presented hereinafter, we modified the basic algorithm of the step-by-step packing method [6] to generate a periodical microstructure. Elastic and plastic properties of grains were scattered about average values within 10%. The property difference is marked using different colors (the darker the grain is, the higher its stress-strain properties are). Then in the numerical simulation we can apply the periodical boundary conditions to simulate loading conditions in the bulk of the material.

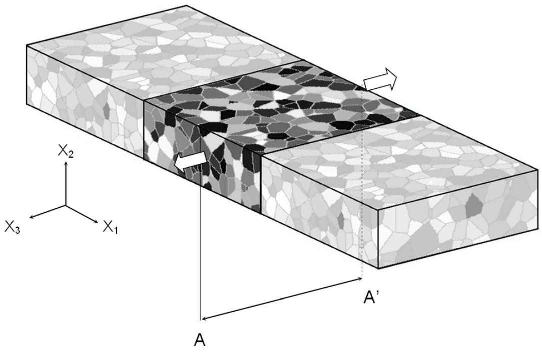
Constitutive equations describing the mechanical response of polycrystalline grains complete the material model. In order to provide realistic material model, the grain shape and size, elastic and plastic properties and strain hardening behavior were defined from experiments for a high-strength steel [5]. Subsequently the three-dimensional model with an explicit consideration of polycrystalline structure is incorporated into a general system of equations of continuum mechanics. The system of equations is complemented by initial and boundary conditions and solved numerically by the finite-difference method.

3 Results and discussion

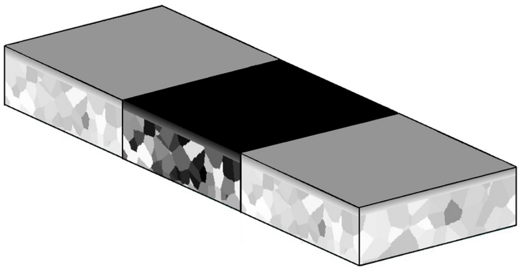
In this section, we apply a computational framework to study the effects of two factors such as modified surface layer width and grain size on deformation-induced surface roughening.

3.1 Roughening in surface hardened polycrystals

The geometry of material models is 200×200×63 μm, it consists of 600 grains (Fig. 1). The average grain size in the base material is 10 μm. In order to design a surface hardened polycrystal (Fig. 1*b*) a structureless layer was grown on the surface of the base material, within the mechanical properties varied linearly from the average characteristics of the base material at the internal boundary to a maximum value on the surface. In calculations the thickness of modified surface layer varied from 5 up to 15 microns. Note, a polycrystalline structure was not introduced explicitly into the model due to the significant difference in grain sizes.



a)



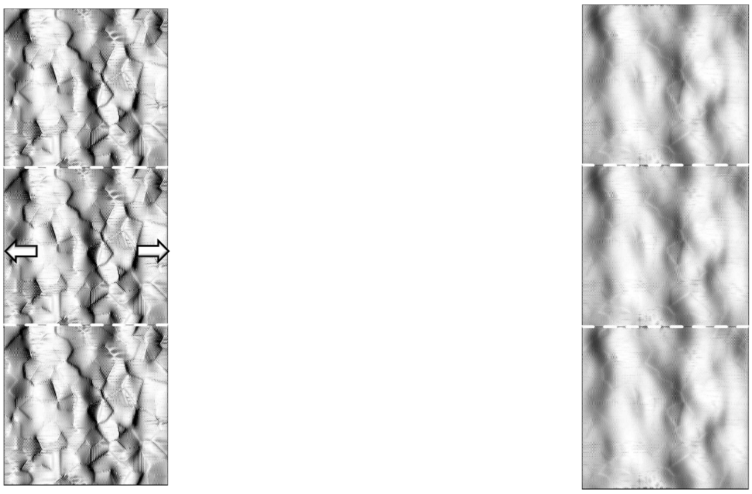
b)

Figure 1: Three-dimensional models of polycrystalline structures without (a) and with (b) hardening. Modified surface layer thickness is of 10 microns (b). Arrows indicate the direction of tension

For the purpose of setting boundary conditions in terms of velocities we introduced the system of coordinates (Fig. 1). Tensile load was applied along the X_3-axis whereas the upper surface was free from external loading and the bottom one was fixed in vertical X_2-direction. Periodic boundary conditions were set at the lateral sides of the specimen.

Numerical simulations were done for unhardened specimen and specimens with modified surface layer of 5, 10 and 15 μm. Note, polycrystalline structure was the same to investigate the influence of hardened surface on the stress-strain state and do not include the geometrical particularities of grains. Calculations have shown that surface relief starts to develop from the very beginning of plastic deformation. Figure 2 demonstrates surface roughening evident as quasi-periodic ridges oriented perpendicular to the axis of elongation. Hills, ridges and valleys involve several grains. Figure 3 shows the corresponding surface profiles taken along the midlines AA' (see Fig. 1a). In the case of unhardened specimen surface folds of different sizes are observed (Fig. 2a, Fig. 3a). Due to interactions and motion of subsurface grains relative to each other small-scale folds are evident in the structure of large-scale ones. The hardened layer characterized by amorphous structure and by absence of grain boundaries noticeably dampens the disturbance associated with displacements of individual grains in the upper layers of the basic material. As the result, the thicker the modified layer, the smoother the surface (Fig. 3b-d).

Let us analyze a distribution of plastic strains. Despite the fact that in all cases the height of the large folds differs but slightly (Fig. 3), surface hardening plays an important role in the deformation behavior of the material. Figure 4 shows a comparison of surface and equivalent plastic strain profiles in the samples with and without modified surface layer. It can be clearly observed that at the same height large folds on the hardened surface are characterized by a smoother displacement gradient than narrow ones on the surface of the base material (cf. Fig. 4 a and b). Since the displacement gradients determine the deformation, the plastic strain localization is much more evident in the case of unhardened specimen (Fig. 4c). Plastic strain is localized at the grain boundaries that form plastic localization bands then. An important implication of the distributions illustrated in Fig. 4 is that the form of roughness structures is of fundamental importance for the development of plastic strain localization.



a) b)

Figure 2: Mesoscopic surface roughening in the unhardened (a) and surface hardened (b) models, $\epsilon = 2.4\%$. Modified surface layer thickness is of 10 microns (b)

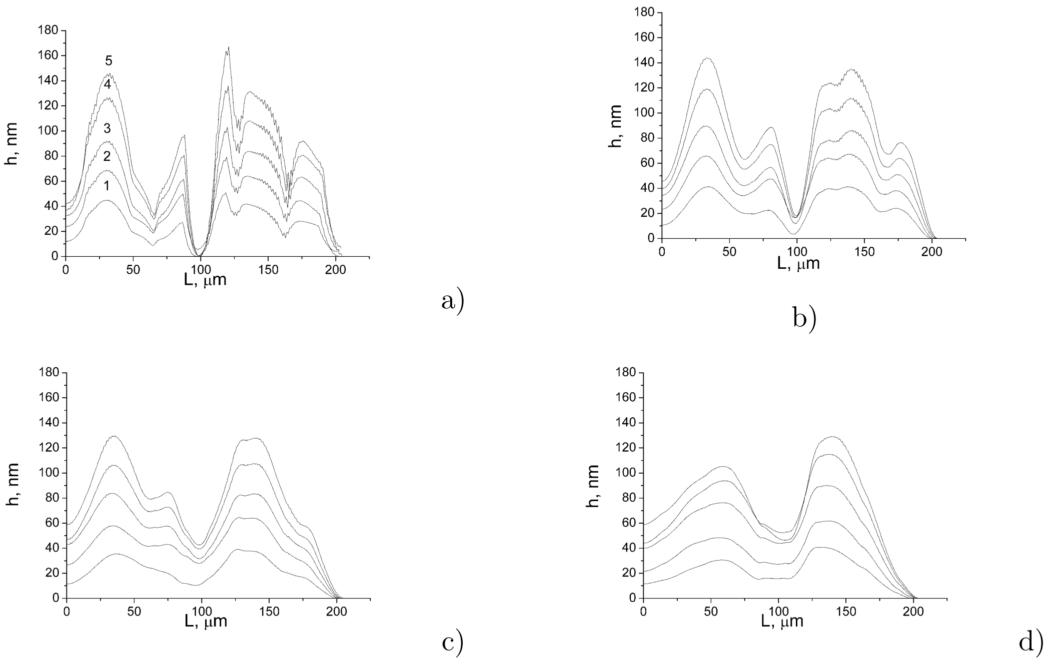


Figure 3: Roughness profiles along the sample midline AA' (see Fig. 1a) corresponding to various strain stages: numbers in subfigure a in ascending order correspond to $\epsilon = 0.5$, 1, 1.5, 2, 2.4%. Modified surface layer thickness is of 0 (a), 5 (b), 10 (c) and 15 μm (d)

3.2 Grain size effect

Computational models of a polycrystalline material with different grain size are illustrated in Fig. 5. In all five cases the model employs 250×250×100 grid with step of 1 μm. The number of grains varied from 450 to 3500, their average grain diameter was 30, 25, 20, 18 and 15 μm respectively. Tension was applied along X_3-axis. The bottom surface was a symmetry plane, the top one was free of an external load and the lateral sides were

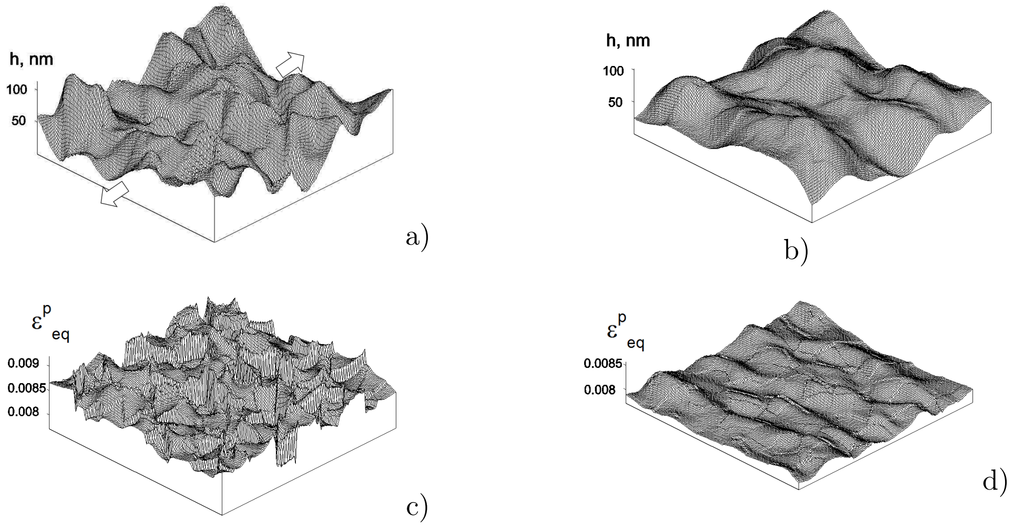


Figure 4: Surface (a, b) and equivalent plastic strain (c, d) profiles on the free surface of polycrystalline samples without (a, c) and with (b, d) modified surface layer under tension up to 0.9%. Modified surface layer thickness is of 10 microns (b, d)

assigned with periodical boundary conditions.

In all cases surface roughening begins to develop early in the loading process in the form of interlacing folds oriented perpendicular to the axis of tension (Fig. 6). Measurement of the fold sizes indicated that height of ridges grows (Fig. 7a-c) and surface roughness develops (Fig. 7d) with increasing average grain size. Figure 7d shows that the maximum roughness parameter R_a was obtained for the structure with the largest grain size referred to in Fig. 5c. Here roughness parameter R_a was introduced in dimensionless form as:

$$R_a = \frac{S_r}{S_f} - 1,$$

where S_r and S_f are rough and flat surfaces, respectively. Also it is supposed that more of grains affect surface roughening in the fine-grained material because the average width of large-scale folds is substantially the same and one can observe more small-scale folds in the structure of those large-scale in the case of the fine-grained material comparably to coarse-grained one.

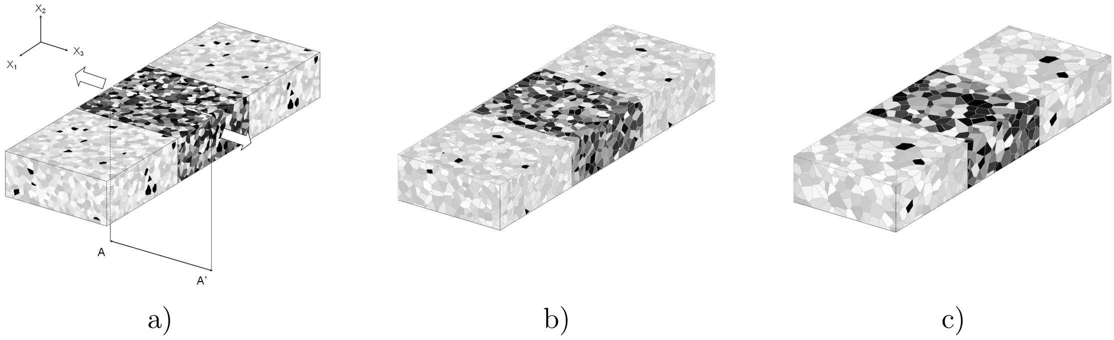
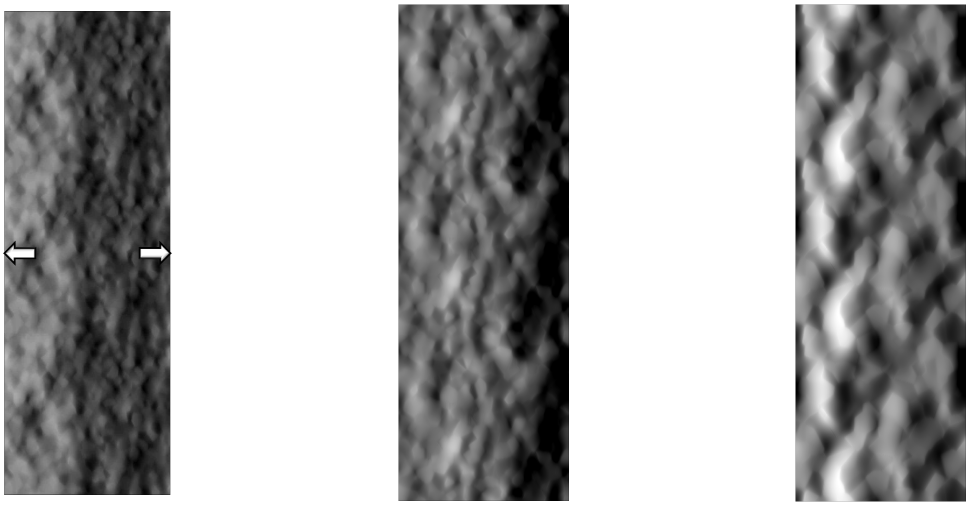


Figure 5: Three-dimensional models of polycrystalline structures with average grain diameter of 15 (a), 20 (b), 30 μm (c)



a) b) c)

Figure 6: Surface patterns formed under tension of 2.9% in specimens with the average grain diameter of 15 (a), 20 (b), 30 μm (c)

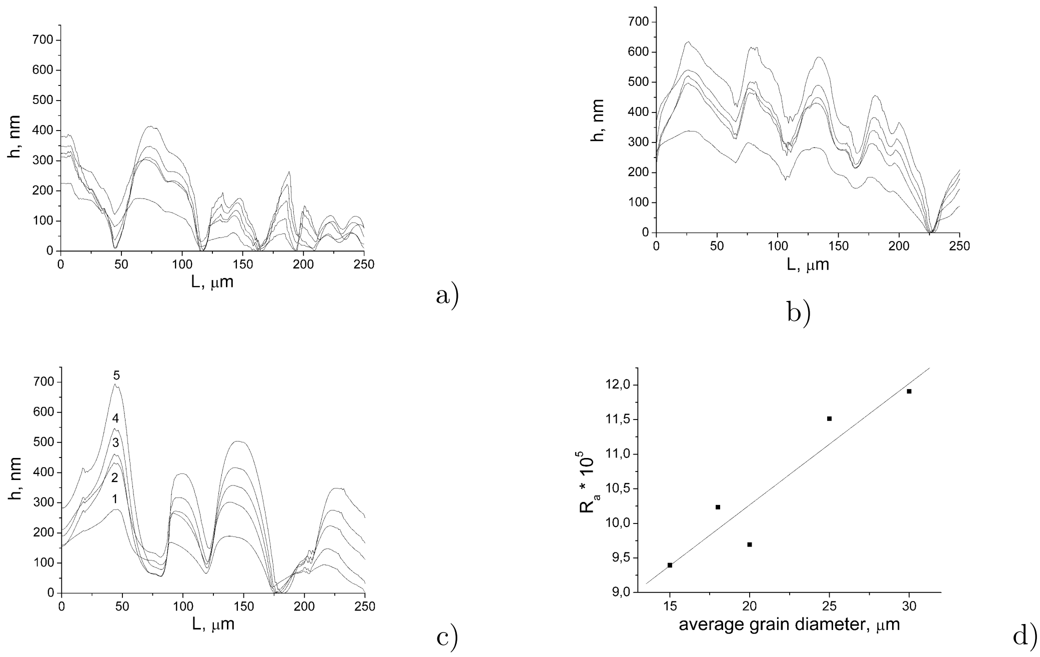


Figure 7: Roughness profiles along the sample midline AA' (Fig. 5a) corresponding to various strain stages: numbers in subfigure c in ascending order correspond to $\epsilon = 0.5$, 1, 1.5, 2, 2.9%. Average grain diameter is 15 (a), 20 (b) and 30 μm (c)

4 Conclusions

Finite-different analysis of steel specimens with different grain sizes and characterized by the presence or absence of a modified surface layer have led to following conclusions.

1) In conditions of constrained deformation, given by periodic boundary conditions, surface roughening evident as quasi-periodic ridges is formed and developed perpendicularly to the axis of tension. Folded structures are formed as a result of displacements of

grain sets relative to each other.

2) As the thickness of the modified surface layer characterized by gradient changes of mechanical properties grows, grain boundaries, which are sources of stresses acting perpendicular to the free surface, are moved away from the surface. As a result, the thicker the modified layer, the smoother the surface.

3) Height of ridges grows and surface roughness develops with increasing average grain size. The maximum roughness parameter R_a was obtained for the coarse-grained structure.

4) Analysis of the stress-strain state of polycrystals considered has shown that localization of plastic deformation is much more evident in the unhardened sample due to the strong displacement gradients.

Acknowledgements

The authors gratefully acknowledge the financial support of Russian Foundation for Basic Research (grant No 12-01-00436-a).

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