Multiscale modelling of damage and fracture processes in nanomaterials

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Abstract. The common multiscale evolution approach to structural modelling of the damage accumulation and fracture processes of submicrocrystalline materials is considered. The method of scanning probe microscopy has been applied to describe the damage evolution on nanoscale. The small-sized plane deformation specimens have been loaded in the tensile device integrated in the scanning probe microscope. The multifractal analysis has been used for the quantitative characterization of in situ deformation of the surface by means of scaling properties. To reveal the mechanism of low-temperature fracture the atomic-force microscopy has been applied to characterize the surface morphology of the stretching deformations of samples fractured at different temperatures.

1. Introduction
The multiscale modelling approach has been actively developed last years [1-6]. First of all, there are many conferences in material and computer sciences taking place where this problem has been discussed [1,3,7]. Some studies have very specific nature like a multiscale modelling of a quantum dot in a semiconductor solid containing a free surface [4], and here the lattice-statics and continuum Green’s functions integrated with classical molecular dynamics are used. The same approach has been used to show significant differences in the deformation behaviour of nanocrystalline nickel with low and high angle grain boundaries [5]. Such works analyse the dislocation activity mainly and are restricted by the method on nanoscale only. Some possibility of multiscale approach was shown as realization of structural and statistical approach [6,7]. In general case the multiscale evolution modelling approach for the damage nucleation and crack propagation in structural submicrocrystalline materials could be presented (see Figure 1). Here the electronic microfractography data means the analysis of micrographs taken by scanning probe or electron microscope, the gage theory means the calibration theory of defects in solids where the Lagrangian of quantum electrodynamics in form $L = \frac{1}{2}(\nabla\psi^\dagger \nabla \psi - \nabla^\mu \nabla^\nu \psi^\dagger \psi) - m \psi^\dagger \psi$ has been used [8]. The procedure of global symmetry localization of this Lagrangian has been used on place to obtain the partial calibration theory [9]. But one of the key feature of the multiscale modelling approach is the obtaining of data of damage nucleation on nanoscale during the deformation in situ. So the device and method of scanning probe microscopy for the in situ deformation of plane specimens has been used. The further quantitative estimation of the scaling features of surface images has been carried out by the multifractal analysis.

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There is only a small number of similar studies known [10], and none of them is applied for the structural alloys and steels.

![Figure 1: Concept scheme of Multilevel Modelling of Fracture](image)

Evolution approach means taking into account the history of the each element on the certain level of structure. The ultimate state of the current level controls the transfer on the next level of structure. The main difficulty is the determination of the ultimate state because it is guided by the number of parameters. But in most cases it is possible to restrict the state to only one control order factor. Here a defect modelling by the calibration theory, not the atomistic simulation, is preferable. The main restriction of the molecular dynamics method is the small size of simulation volume, a necessity to simplify the quantum dependences for electron configuration and difficulty in connection to upper scale level [1-3]. The defect modelling on different structural levels allows simulating behaviour of material under the wide range of external influences without abovementioned faults. On the concept scheme the main points and methods used have been shown.

### 2. Materials and methods

As it has been mentioned beforehand it is the necessary to obtain the data of damage nucleation on nanoscale during the deformation in situ. So the device of scanning tunnelling and atomic-force microscopy for the in situ deformation of plane specimens has been developed and used. The first specially designed device has been produced by “Proton-MIET” company (Zelenograd, Moscow Distr.) as a combination of a scanning tunnelling microscope with a strain gauged loading setup. Recent experiments were performed using the second device containing the loading setup and the removable scanning platform with atomic-force probe suitable for structure experiments in different conditions (see Figure 2). Both microscopes have scanning platform (SP-STM and SP-AFM) construction. However the massive antivibration table and removable scanning platform in SP-AFM construction provide higher resolution and images of high quality are to be obtained much easy. For the small-size specimens the ultrafine-grained steel produced by the method of intensive plastic deformation (equal-channel angular pressing) has been used [11].
In addition to revealing the mechanism of metal fracture under low temperatures, the fracture surfaces of construction elements and sample models are being studied. Optical and scanning tunnelling microscopy of fractured surfaces of samples under different external environments and after different types of influences on the metal has been realized, and a complex of metallographic and microstructure studies has been carried out also. So the small-size specimens were saturated at high temperature and high pressure by hydrogen. It is necessary to define the microdefects size distribution function, its shapes and average concentration depending upon the static and corrosion influence, for the obtaining the probabilistic damage estimations.

![Figure 2](image1.png)

**Figure 2.** View of (a) loading device and fixed plane tensile specimen on antivibration table and (b) SP-AFM probe placed on the table with specimen.
3. Results and Discussion

Using the method of scanning tunnelling microscopy the fracture of low-alloys steel samples was explored. The samples were saturated preliminarily by the hydrogen at the 400°C temperature and 10 MPa pressure conditions and tested for the delayed fracture sensibility. As the size of investigation area is 2.6×2.6 μm, the height of microrelief is achieved 0.2 μkm. The typical sizes of the secondary microcracks – depth is 0.2 and width is 0.3 μm. The indication that the cracks are propagating by the mechanism of nucleation and coalescence of such microdefects as micropores and microcracks is obtained here. It is agree with the known visualisation model of fracture [12].

The study of ultimate states of material is directly connected to the lifetime numerical estimation of constructions manufactured from widely used and new materials. The last investigations in this directions are linked to the study of influence of grain boundaries and interfaces, particularly, impurity segregations on grain boundaries, on the deformation and fracture of polycrystalline and nanostructural materials. By means of scanning tunnelling microscopy the “in situ” investigation of the evolution of surface damage during the deformation of small-sized specimens of the experimental cold-resistant steel was conducted. The fitted 4.5 kN loading device and the electronic tunnelling probe with 20×20×2 μm scanning field has been used. The results of scanning of the grain boundary during the deformation (the deformation curve is indicated on figure 3) have been shown on figure 4. It is seen that before the extensive macroscopic plastic deformation the surface relief change and the microcracks is appeared on the 3D-images and profiles. The damaging has been numerically estimated by the methods of multifractal analyses of the scanned images [7].

The calculation of parameters of the multifractal spectrum has been performed for the equal areas (100×100 pixels or 580×580 nm) in grain boundary zone for the (a) initial state, and for the steps on deformation curve - (b) 1500, and (c) 1650 N (see fig.4). According to the initial surface image and multifractal parameters obtained the initial roughness is high and during the deformation is growing (see the table 1). The changing of fractal dimensions – the Hausdorff $D_0$, the correlative $D_1$ and the informational $D_2$ – is same for the deformation surfaces.

![Figure 3. View of in situ loading control curve in electron probe scope.](image-url)
Figure 4. The 2D and 3D-images of the probed surface at grain boundary during the deformation in situ, (a) in initial state, and at the steps on deformation curve - (b) 1350, (c) 1500, and (d) 1650 N.

Table 1. The multifractal spectra parameters of deformation surfaces in situ.

| Parameter | On initial surface | On loaded at 1500 N | On loaded on 1650 N |
|-----------|--------------------|---------------------|---------------------|
| D0        | 2,389              | 2,455               | 2,376               |
| D1        | 2,277              | 2,297               | 2,258               |
| D2        | 2,206              | 2,218               | 2,179               |
| K         | 1,505              | 2,518               | 1,799               |
| Δ         | 0,325              | 0,462               | 0,433               |
| f(40)     | 0,528              | 0,107               | -0,292              |

Concerning the structure of the investigated surfaces, it has been the hidden periodicity measure $K = D(-40) - D(40)$ that estimate the regularity of surfaces, and measure of order $Δ = D(1) - D(40)$. The higher values of thus measures mean the more periodic components the surface contains. The last parameter of the multifractal spectrum reveals the porosity of surface, and during the deformation it is monotonic decreasing.

The atomic-force microscopy of the morphology of surface stretching deformations of samples fractured at different temperatures has been carried out also. Microstructure peculiarities of damage accumulation and the character of nanostructured steel fractures at low temperatures were revealed. The microstructural aspects of deformation and fracture of nanostructured steel at low temperature (−60°C) are considered. By the methods of optical and atomic-force microscopy the deformation surfaces of the fractured tension probes was studied. The fracture character changes (from a brittle cleavage to a ductile shear) at low temperatures, it has been shown to be associated, on the one hand, with a fuzzing of grain boundaries during angular pressing with solid structural phases and, on the other hand, by the replacement of the prevalent plastic deformation carriers [13].

4. Summary

According to the common multiscale evolution approach to structural modelling of the damage accumulation and fracture processes of submicrocrystalline materials the method of scanning probe microscopy has been applied to subscribe the damage evolution on nanoscale. The small-sized plane specimens have been loaded in the tensile device integrated in scanning probe microscope. For the
quantitative characterization of the damage of in situ deformation surface the multifractal analysis has been used. To reveal the mechanism of low-temperature fracture the atomic-force microscopy of stretching deformation surfaces has been applied. The fracture character changes have been shown to be associated with a fuzzing of grain boundaries and by the replacement of prevalent plastic deformation carriers.

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