MULTISCALE MODELING OF DEFORMATION PROCESSES IN SITU

Valeriy V. Lepov[1], Boris A. Loginov[2]

[1]Larionov's Institute of Physical-Technical Problems of the North SB RAS, Yakutsk, Russia
[2] Moscow Institute of Electronics (Technical University), Moscow, Russia

Introduction

The multiscale modeling 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 modeling 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 analyze 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].
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. There is only a small number of similar studies known [8], and none of them is applied for the structural alloys and steels.

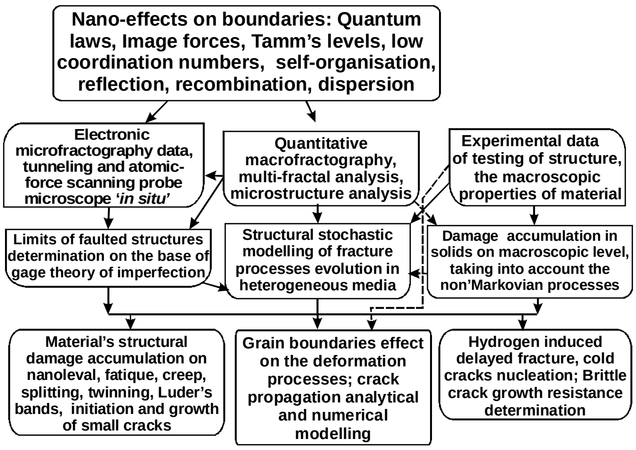

Fig.1 Concept scheme of multiscale modeling

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.

Experimental

As it has been mentioned beforehand it is necessary to obtain the data of damage nucleation during the deformation in situ on nanoscale. 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 tunneling 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).

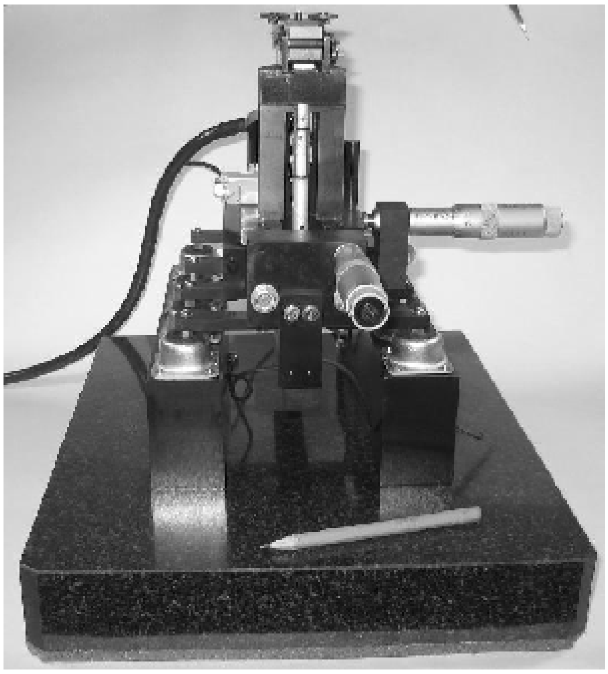

Fig.2 View of the AFM with loading device

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 [9].

Results and Discussion

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 D0, the correlative D1 and the informational D2 – is same for the deformation surfaces.

Table 1 The multifractal spectre 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.

Conclusion

The new multiscale non-Marcov evolution modeling approach for damage accumulation and fracture processes of polycrystalline and ultrafinegrained materials is proved by experimental results on nanoscale. Parameters of the model estimated by electronic atomic-force scanning probe during the deformation “in situ”. The non-Marcov evolution in new approach means taking into account the history of each element on certain level of structure. The ultimate state of the current level control the transfer on the next level of structure. The main difficulty of traditional multiscale modeling is the determination of the ultimate states due to the lot of guide parameters. New approach presumes possibility to restriction the current state of material to only one control order factor. Well-known main restrictions of the molecular dynamics method are the small size of simulation volume, a necessary to simplify the quantum dependences for electron configuration and connection to upper scale level difficulty. The new approach of defect behavior modeling allows simulating of material under the wide range of external influence, including low and high temperature and other environmental effect, almost without any faults.

Acknowledgements

The support of Russian Foundation for Basic Research (Grant 09-01-98511) and Presidium of Russian Academy of science (Project 27.40) is gratefully acknowledged. Author thanks Ivanov A.M., senior researcher of IPTPN SB RAS to help in ultrafine-grained steel specimen preparation.

References

1. Sih G C, editor 2007 *Multiscaling in Molecular and Continuum Mechanics: Interaction of Time and Size from Macro to Nano* (London: Springer)
2. Loehnert S, Belytschko T 2007 Int. J. Num.. Meth. Eng 71 1466
3. Meguid S A, Wernik J Multiscale modelling of the nonlinear behaviour of nano-reinforced composite interfaces 2009 Proceedings of the International Conference IRF’2009 ed J F Silva Gomes and Shaker A. Meguid pp 5-6
4. Tewary V K, Read D T 2005 Nanomechanics of Materials and Structures 342 89
5. Vaithyanathan V, Wolverton C, Chen L Q 2002 Phys.Rev.Lett. 88 125503
6. Lepov V, Ivanova A, Achikasova V, Lepova K 2007 Key Engineering Materials 345-346 809
7. Lepov V V, Ivanova A A, Achikasova V S, Lepova K Ya 2008 Structural-statistical Aspects of the Damage Accumulation and Fracture Modelling ICF Interquadrennial Conference. Fracture Mechanics in Design of Fracture Resistant Materials and Structures ed R V Goldstein
8. Bagrov D, Yaminskiy I 2008 Nanoindustry 5 32 (in Russian)
9. Ivanov A M, Lukin E S, Petrova N D, Vashenko S S 2010 Reviews on advanced materials science 25 203