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Multiscaling of Lattice Curvature on Friction Surfaces of Metallic Materials as a Basis of Their Wear Mechanism

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Abstract—A comprehensive structural study has been performed to explore deformation and wear debris formation on friction surfaces of metallic materials. A hierarchy of structural scales of plastic deformation and failure during wear has been established. The nanoscale plays the major role in the hierarchical self-organization of multiscale debris formation processes. On this scale, bifurcational interstitial states arise in zones of local lattice curvature, with plastic distortion and motion of nonequilibrium point defects which determine the nonlinear dynamics of structure formation and wear of surface layers. Nonequilibrium vacancies on lattice sites form microporosity through the coalescence mechanism under plastic distortion. The microporosity is a precursor of meso- and macroscale plastic shearing that defines wear debris formation.

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Keywords: multiscaling, friction, wear, lattice curvature, plastic distortion, wear debris

1. INTRODUCTION

This paper is based on the physical mesomechanics concept of self-organization principles in multiscale hierarchically organized systems [1–5]. It provides convincing evidence on the relationship of material wear mechanisms on friction surfaces to multiscaling of lattice curvature in surface layers of friction contacts.

The dislocation mechanism of deformation under uniaxial tension of metallic materials governs their high ductility. This is due to the fact that primary shear in a loaded specimen occurs in a 2D planar subsystem (surface layers and grain boundaries in polycrystals) that lacks translational invariance. Flows of structural transformations in grain boundaries are well known as grain boundary sliding. It gives rise to couple stresses that act on grains. In accordance with the law of conservation of angular momentum, opposite-sign rotational modes of dislocation deformation must occur in grains. The generation of dislocations at the interface between the 2D planar and 3D crystal subsystems as well as the vortex-like propagation of dislocations in the crystalline material in fact inhibit the nonlinear wave of grain boundary sliding. In these conditions, the following relation is valid:

$$\sum_{i=1}^{N} \text{rot} J_i = 0, \qquad (1)$$

where J_i are the defect fluxes on the i-th structural scale level. All couple stresses are compensated in the material in these conditions, and the crystal lattice preserves its translational invariance. As long as Eq. (1) holds true, the material is ductile.

An absolutely different loading scheme is observed in material surface layers under friction. Couple stresses in friction contact areas induce lattice curvature of friction surfaces. Interstitial lattice sites are the places where new minima of many-body interatomic interaction potentials appear [3, 5] and structural turbulence through plastic distortion becomes possible [6]. Dynamic rotations occur in the surface layer structure, with a high concentration of athermal vacancies on the lattice sites that have undergone plastic distortion. The coalescence of athermal vacancies leads to microporosity formation on the boundaries of dynamic rotations, to microcrack nucleation, and wear debris formation.

The wear-induced failure of the surface layer is a rotational mechanism that develops as a multiscale hierarchically organized process. Wear debris flake off in a material with broken translational invariance, wherein very thin surface layers become nanostructured. Multiscaling of lattice curvature lies at the basis of material wear on friction surfaces.

This paper presents a complex structural investigation of material wear mechanisms and patterns based on the physical mesomechanics concept of multiscaling of lattice curvature on friction surfaces.

2. NON-EUCLIDEAN MODEL OF PLASTIC DEFORMATION AND WEAR MECHANISM OF SURFACE LAYERS IN FRICTION PAIRS

Earlier, we wrote about the vortex-like development of plastic deformation on friction surfaces [7]. It breaks translational invariance and gives rise to lattice curvature in the surface layer (Fig. 1). The rotational plastic deformation mechanism should be described by the non-Euclidean model of Myasnikov and Guzev [4] in which tensors of curvature $^{*}R^{\kappa}_{ijq}$, torsion $^{*}C^{\kappa}_{ij}$, and nonmetricity $K_{\kappa ij}$ are introduced. This is a way to introduce the geometry of the affine-metric space for a deformed crystal which appears to be stable with slight changes in the tensors $^{*}R^{\kappa}_{ijq}$, $^{*}C^{\kappa}_{ij}$ and $K_{\kappa ij}$. Note that all the given tensors of the affine-metric space are zero in a translationally invariant crystal.

In the literature, the tensors $^{*}R^{\kappa}_{ijq}$, $^{*}C^{\kappa}_{ij}$ and $K_{\kappa ij}$ are conventionally correlated with various deformation defects, such as disclinations, dislocations, and point defects [8]. The problem of wear is described in many papers on the basis of dislocation theory. However, dislocations are microscopic translational defects of a translationally invariant lattice, while rotational wear mechanisms develop in the scale hierarchy of wear debris [9]. In this case, the most important functional role in the wear mechanism belongs to the nanoscale level that was not earlier considered in wear physics and wear mechanics.

The mesomechanics of multiscale hierarchically organized systems has introduced nanoscale point defects [2, 3, 5] that describe plastic distortion in the fields of atomic displacements to the interstitial sites of lattice curvature zones. The model of nanoscale point defects in lattice curvature zones in a deformed polycrystal is depicted in Fig. 2. Primary flows of structural transformations in a deformed polycrystal occur in a 2D planar subsystem (surface layers and polycrystal grain boundaries) that lacks translational invariance. The distribution of normal stresses σ_n on the boundary of misoriented polycrystal grains is described by a sinusoidal function, i.e., zones of tensile and compressive stresses σ_n alternate [10, 11]. This grain boundary sliding mechanism causes the formation of clusters of positive ions in the zones of tensile normal stresses which are screened by electron gas from nearest neighbors in the near-boundary region of a 3D crystal grain. A decrease in the concentration of free electrons between ions *C-D*, *E-F*, *G-H* leads to an increase in their interionic spacing and the appearance of a local gap in the electron energy spectrum [12]. This is equivalent to the appearance of a quantum dot in the system which generates its "impurity" electronic eigenstates in the local energy gap of the electron energy spectrum. As a result, bifurcational minima of the many-body interaction potential appear in the interstitial sites *C-D*, *E-F*, *G-H*. Atoms in pairs *C-D*, *E-F*, *G-H* will be

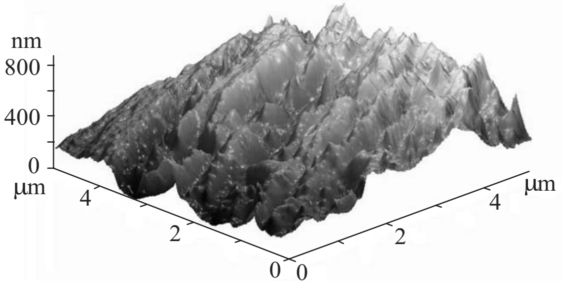

Fig. 1. Nickel surface with high-curvature nanostructured folds in the friction contact zone of nickel. Atomic force microscopy [7].

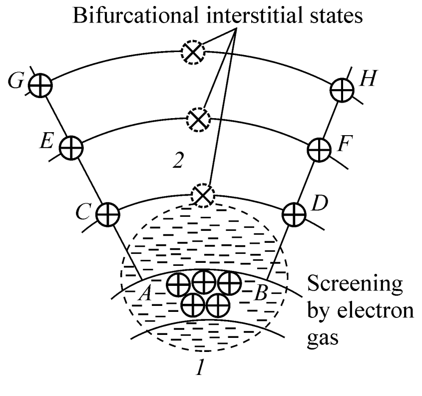

Fig. 2. Generation of bifurcational interstitial states in local lattice curvature zone, *AB*—clusters of positive ions at the boundary of grains *1* and *2* [3].

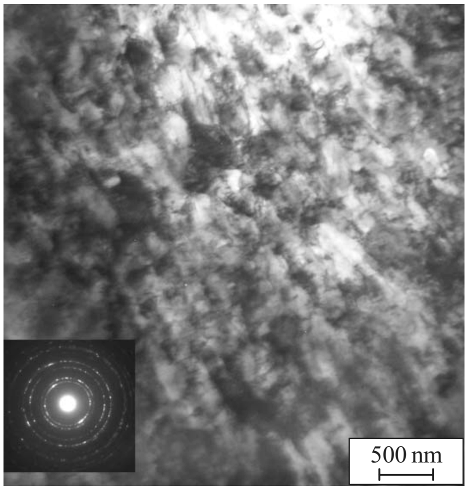

Fig. 3. Nanostructural state of nickel surface for the friction time $t = 7$ h. Transmission electron microscopy.

displaced during shear deformation with plastic distortion in the zone of bifurcational interstitial minima of the many-body potential, giving rise to a vortex-like local plastic flow. An expression for the vorticity of localized plastic shear, derived by Egorushkin [13], reads:

$$\chi_{\nu}^{\beta} = \varepsilon_{\mu\chi\delta}\frac{\partial(E_{\nu}^{\beta} - P_{\nu}^{\beta})}{\partial x}\frac{C_{\alpha\beta}^{\mu\nu}}{E}, \qquad (2)$$

where $\varepsilon_{\mu\chi\delta}$ is the Levi-Civita symbol; the bracketed expression reflects shear stress relaxation through plastic distortion P_{ν}^{β} in local lattice curvature zones. In order for lattice curvature to be taken into account within the entire volume of a deformed solid, a nonlinear mechanics of plastic deformation and fracture must be developed.

The generation of bifurcational interstitial states and plastic distortion effects are enhanced under severe plastic deformation, when lattice curvature is highly pronounced [14–17]. Studies on structure refinement in materials subjected to equal channel angular pressing [14, 15] and friction stir welding [17] place particular focus on the problem of material wear. Equal channel angular pressing induces lattice curvature over the entire workpiece cross section, with plastic distortion in interstitial lattice sites accompanied by the formation of a large amount of vacant lattice sites. Their multiscale coalescence causes initial structure fragmentation on the meso- and nanoscale. Friction stir welding also leads to material fragmentation on friction contacts and plastic distortion with the formation of athermal vacancies on lattice sites, due to which structural elements are cold welded together.

Such multiscale processes occur on friction surfaces with material fragmentation, formation of athermal vacancies on friction contacts, their coalescence, and flaking of wear debris. In very thin surface layers of materials, nanostructure (Fig. 3) and microporosity form (Fig. 4). Let us consider in more detail these processes on friction surfaces within the non-Euclidean model framework.

3. SELECTIVE FAILURE MECHANISM OF THE SURFACE LAYER IN METALLIC MATERIALS UNDER FRICTION

As the broken translational invariance in the material on friction contacts gives rise to lattice curvature of the surface layer, a crucial task is to assess this characteristic. In our earlier papers [18, 19], we did it by measuring

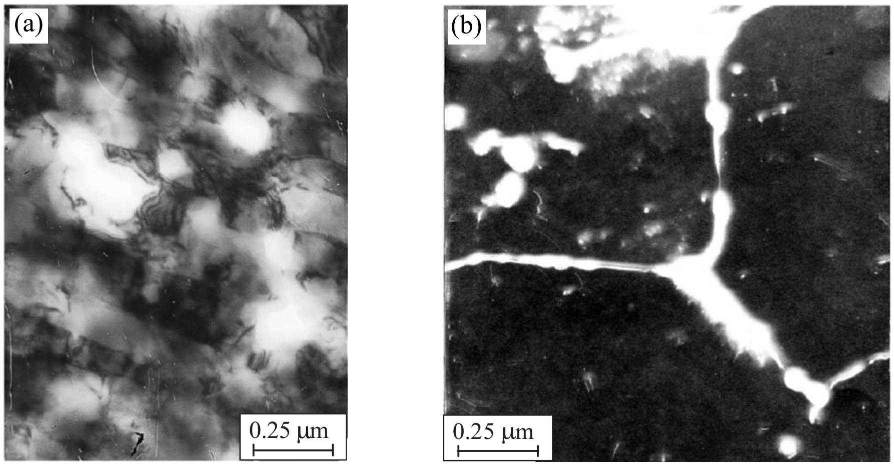

Fig. 4. Microporosity formation inside and at the boundary of mesosubstructural blocks in the surface layer of friction contact in nickel [19].

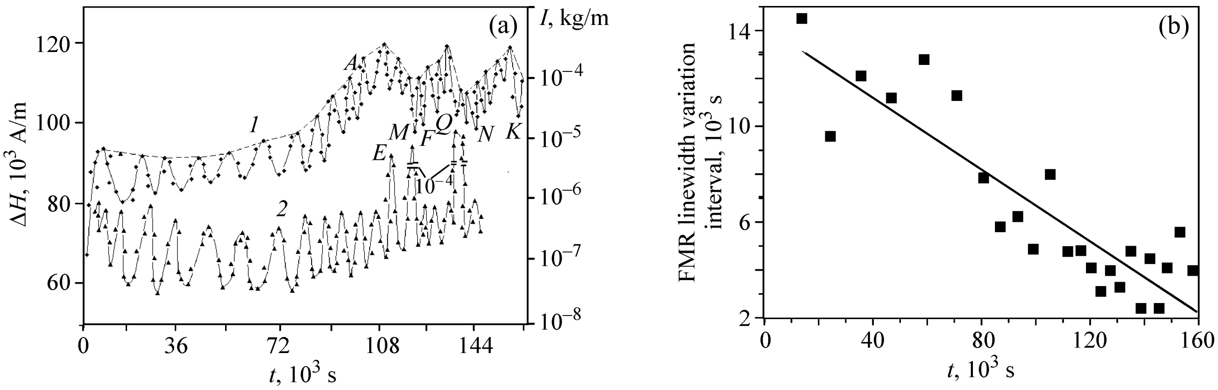

Fig. 5. Ferromagnetic resonance (FMR) linewidth ΔH (*1*) and wear intensity I (*2*) versus friction time t, $P = 84$ kPa; $v = 0.5$ m/s; TsIATIM-201 grease, pin (Ni)-on-disk (Mo) friction scheme [18, 19] (a); duration of ΔH variation cycles for the parameter given in Fig. 5a versus friction time.

the ferromagnetic resonance linewidth in wear of specimens of various ferromagnetic materials. The variation kinetics of the ferromagnetic resonance linewidth of nickel ΔH and wear intensity I under friction is represented in Figs. 5 and 6. The friction surface was lubricated with TsIATIM-201 grease [20]. As is seen from Fig. 5, the ferromagnetic resonance linewidth (curve *1*) cyclically increases and decreases, bearing witness to a cyclic lattice curvature variation in the surface layers of friction contacts. Of fundamental importance is that ΔH cyclically varies simultaneously with wear intensity I (curve *2*). The wear intensity maxima match well with the lattice curvature minima. In other words, flaking of wear debris is accompanied by a sharp decrease in their lattice curvature. At the same time, the lattice curvature increase in the surface layers of friction contacts is accompanied by a sharp decrease in wear intensity. This means that flaking of wear debris (i.e., surface layer failure) starts at the achievement of a critical lattice curvature in the surface layer. Since the maximum ΔH value corresponds to the maximum plastic distortion at which the concentration of vacant lattice sites is maximum, material fragmentation in the surface layer and separation of its fragments in the form of debris are explainable. Multiscaling of lattice curvature determines a wide size range of wear debris [14]. The coalescence of vacant lattice sites in the surface layer takes place in a sinusoidal stress field at the interface between the highly curved surface layer and the crystalline substrate. Segal et al. [14] found two maxima for the wear debris sizes. In a heterogeneous medium, there can be more maxima.

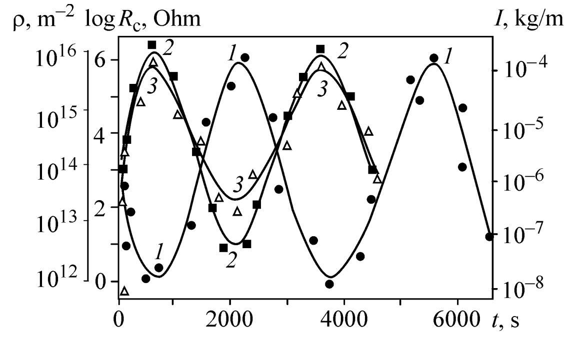

Fig. 6. Wear intensity I (*1*), contact resistance R_c (*2*), and density of deformation defects (*3*) versus friction time t.

Figure 6 illustrates that the contact electrical resistance R_c on the lubricated friction surface oscillates. This effect correlates well with the oscillation of ΔH, i.e., the lattice curvature value of the surface layer, and with the wear intensity oscillation. The maximum wear intensity corresponds to the minimum contact electrical resistance. In other words, flaking of wear debris from the surface layer breaks the lubricant film and uncovers the juvenile surface of the metallic substrate. The contact electrical resistance sharply decreases in this case. Thus, the laws of cyclic variation of ΔH, I and R_c in Figs. 5 and 6 are compelling evidence to the selective failure mechanism of fiction contact surfaces.

Crucial to the wear mechanism is the multiscale lattice curvature of the surface layer. This is confirmed by the progressive increase in the oscillation frequency of the ferromagnetic resonance linewidth ΔH and wear intensity I with time during wear, which is illustrated in Fig. 5a. The oscillation frequency of ΔH and I is associated with the debris size reduction. This has been well

Table 1. Reduction of average debris size with wear time [19]

Wear time, 10^3 s	25.2	93.6	126.8
Average debris size, μm	4.0	3.2	2.5

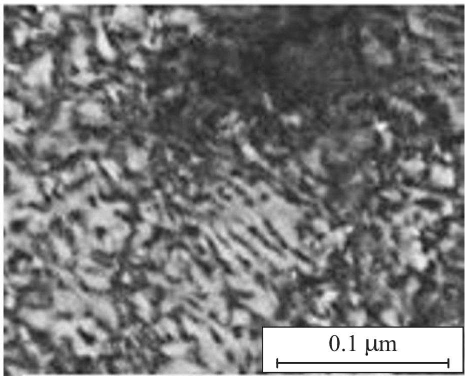

Fig. 7. Microfolded structure in the surface layer of friction contact in nickel.

corroborated by experiments, whose data are provided in Table 1.

As new structural states arise in interstitial sites of lattice curvature χ [3, 5], the increase of χ leads to the enhancement of the plastic distortion effect. Atoms become capable of moving from lattice to interstitial sites in lattice curvature zones and of arbitrarily changing the vortex-like motion trajectory. This makes for debris size reduction.

4. STRUCTURAL STATE EVOLUTION IN THE MATERIAL SURFACE LAYER UNDER FRICTION

A folded structure with a fold height of up to ~300 nm is formed in the deformed surface layer (Figs. 3 and 7). Clearly, a translationally invariant crystal cannot produce the folded structure. Hence the surface layer becomes nanostructured, which is illustrated by the circular diffraction pattern in the insert in Fig. 3. Plastic distortion in the zones of high lattice curvature leads to a high concentration of vacant lattice sites. Their coalescence governs microporosity formation (Fig. 4) and microcracking (Fig. 8).

Figure 8a clearly demonstrates how wear debris form in the surface layer. Plastic shear and cleavage crack *AB* are generated at the tip of localized shear band *A*, in compliance with fracture mechanics predictions [21]. The cleavage crack experiences accommodating rotation along direction *BC* through plastic distortion and coalescence of vacant lattice sites. Such crack rotations progress along its propagation path and end in the separation of a wear particle. An example of crack propagation along a nanoporous localized shear band is illustrated in Fig. 8b [22].

Another example of wear debris formation in the surface layer of a polycrystal under friction is given in Fig. 9. A complex stress state of material in triple grain junction *Q* induces two effects. First, microporosity forms in polycrystalline grains. Second, grain boundary sliding induced by the stress concentrator in the triple grain junction causes a clockwise rotation of block *P* in grain *1*. A large stress concentrator is formed in corner point *G* of grain *2* during grain boundary sliding. Pronounced microporosity develops in its vicinity in grain *1*. The stress concentrator in corner point *G* initially generates a localized shear band in the microporous structure, where micropores coalesce into a microcrack. Microporosity develops on all boundaries of triple junction *Q*, thus providing for the separation of block *P* in grain *1* as a wear particle.

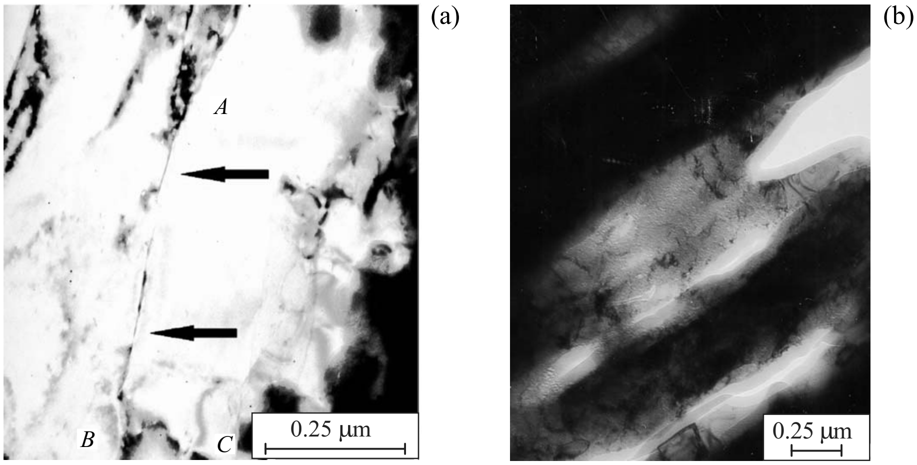

Fig. 8. Nucleation of a cleavage crack at the tip of localized shear band *A* and its rotation in zone *BC* through micropore coalescence (a); macrocrack propagation along nanoporous localized shear band (b) [22].

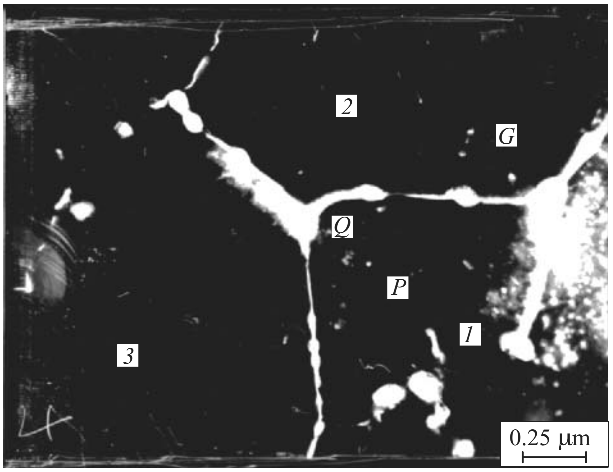

Fig. 9. Rotational mechanism of the formation of wear particle *P* in the surface layer of friction contact in nickel [19].

The vortex-like character of wear debris separation from the substrate on the mesoscale must be compensated by opposite-sign rotational modes in the surface layer on the microscale (the law of conservation of angular momentum). This is clearly demonstrated by transmission electron microscopy (Fig. 10). As is seen from Fig. 10a, a cellular dislocation substructure is formed in the surface layer of polycrystalline nickel prior to wear debris separation during friction. It is specific that under uniaxial tension of nickel specimens at room temperature (Fig. 10b) transmission electron microscopy reveals no dislocation splitting in the cellular dislocation substructure, while on friction surfaces dislocation splitting is very pronounced (Fig. 10a). The vortex-like motion of material blocks is accommodated by individual split dislocations that clearly define the rotation profile of the material block (Fig. 10a).

Abnormally low stacking fault energy of highly split dislocations in the surface layers of friction contacts bears witness to high thermodynamic nonequilibrium of the friction surface material. This can be only due to a high lattice curvature of the material in which plastic distortion occurs and athermal vacant lattice sites reach a high concentration. Lattice nanostructuring takes place in the material with the appearance of a developed system of nanograin boundaries, making possible the formation of a fine folded structure on the friction surface (Fig. 7). The elastic moduli of such a “loose” crystalline structure are very low because the crystalline state of the material is close to decomposition and its Gibbs thermodynamic potential is close to zero [23]. In these conditions, the cores of highly split dislocations move in a viscous manner with changes in the folded profile of the nanostructured surface layer material. In other words, the highly split dislocations depicted in Fig. 10a do not slide but form an elastic-plastic nanoscale folded structure of the nanostructured surface layer of friction contacts.

The formation of folded profile in the surface layers of friction contacts leads to the formation of micropores in localized shear bands whose coalescence causes microcracking (Fig. 11). This exemplifies the initial stage of wear debris formation in a highly nonequilibrium material of friction contact on the mesoscale.

Microporosity formation in localized shear bands as a precursor of ductile fracture in a deformed material was earlier discussed by Tekoglu et al. [24]. Emphasize that this effect is determining in the material wear mechanism

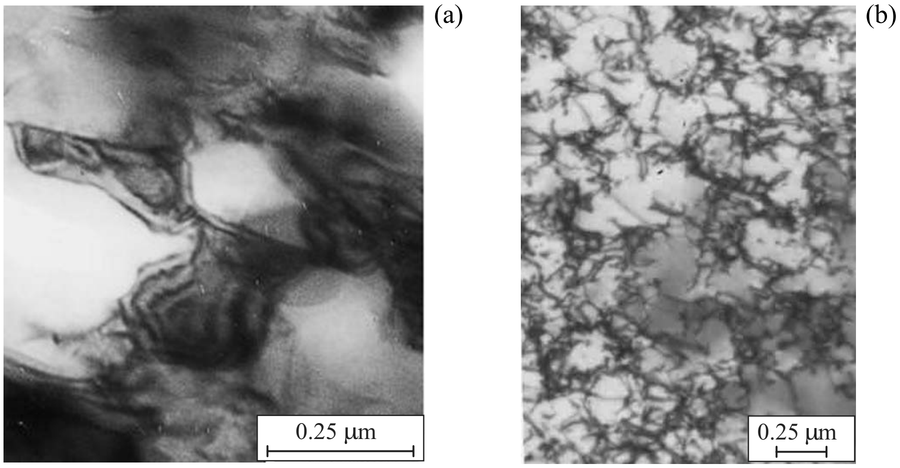

Fig. 10. Nucleation of highly split dislocations of accommodation origin on the contour of subgrain *P* in its rotational deformation (a); cellular dislocation substructure under tension (b) [19].

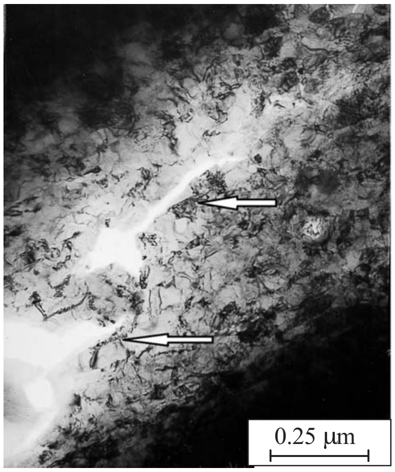

Fig. 11. Initial stage of wear debris contour formation in the surface layer of friction contact in nickel [19].

on friction surfaces where wear debris formation must be described only within the framework of nonlinear fracture mechanics.

The results represented in Figs. 8–11 strongly confirm that the vortex-like plastic flow on friction surfaces as well as lattice curvature formation, plastic distortion effect, microporosity formation and microcracking in these surfaces lie at the basis of the multiscale mechanism of wear debris formation and their selective separation from the substrate.

5. STRUCTURAL SCALE HIERARCHY OF PLASTIC DEFORMATION AND FAILURE IN MATERIAL WEAR ON FRICTION SURFACES

Tables 2 and 3 represent a hierarchical self-organization of structural scales of plastic deformation and fracture in material wear on friction surfaces. Multiscaling of the wear process is based on the structural transformation nanomechanisms on friction surfaces associated with lattice curvature. Of fundamental importance is the physical mesomechanics concept [3] about the generation of bifurcational structural states in interstitial sites of lattice curvature which govern the plastic distortion effect. Atoms of substitutional elements in these zones can move from lattice sites to interstitial ones, giving rise to elastoplastic rotations of arbitrary configuration. A thin surface layer in friction contacts becomes nanostructured and deforms through the motion of nonequilibrium point defects, including interstitial sites and the plastic distortion effect. Nonequilibrium vacancies in the lattice sites from which atoms moved to interstitial sites coalesce and form nano- and microporosity as a precursor to ductile fracture of the material [24].

Then, the process develops in a blow-up mode simultaneously on the micro-, meso- and macroscopic structural scales. The concept of blow-up fracture of solids was put forward by Malinetskii and Potapov [25]. The blow-up fracture is especially pronounced during wear, wherein surface layers in friction contacts turn to be nanostructured and their structure is highly nonequilibrium. Plastic shearing in nanostructured materials occurs under the action of maximum tangential stresses [26, 27]. Couple stresses from the elastically loaded substrate act on the plastically deformed surface layer in friction contacts. This governs its vortex-like plastic flow in the structural turbulence scheme [6]. The microporosity formed in the surface layer and the plastic distortion effect determine a wide size range of wear debris and a very high rate of their separation from the substrate. Self-organized structural transformations on the nano- and microscale give rise to a highly nonequilibrium structural state of the nanostructured surface layer of friction contacts (Table 2). Localized shear bands in the structural turbulence scheme form different-size wear particles that easily separate from the substrate owing to the developed microporosity and plastic distortion (Table 3).

Accommodating plastic shears in in-depth substrate layers form their defect substructure that reduces the oscillation period of the ferromagnetic resonance linewidth ΔH and wear intensity I (Fig. 5a). This self-organization requires additional research. However, this paper has properly elucidated the multiscaling effect in multiscale hierarchically organized wear processes on friction surfaces.

6. CONCLUSIONS

The wear mechanism of metallic materials in friction pairs has been analyzed based on the multiscale approach of physical mesomechanics. It was shown that the wear mechanism cannot be described using conventional concepts of fracture mechanics and dislocation theory for translationally invariant crystals. Surface layers in friction contacts become nanostructured, being in a highly nonequilibrium state. A high lattice curvature forms in these layers, which is the source of unconventional structural transformations: plastic distortion of atoms from lattice to interstitial sites; formation of nonequilibrium vacancies on lattice sites in lattice curvature zones; coalescence of nonequilibrium vacancies with microporosity formation and microcracking in the field of couple stresses that arise in noncrystallographic localized shear bands during their interaction with the immobile substrate.

The development of lattice curvature and related nonlinear structural transformation mechanisms are

Table 2. Multiscale selective wear mechanisms (nano and micro)

Structural scales of plastic deformation and failure			
Nano	Micro		
Deformation	Deformation	Fracture	Wear
Local lattice curvature Bifurcational interstitial states Plastic distortion Nonequilibrium vacancies Coalescence of nonequilibrium vacancies Nanopores Nanodiscontinuities	Formation of clusters of deformation defects ($\sim$0.1 μm) Banded structures in slip bands (0.1–1.0 μm in size) Highly dispersed nanostructured layer with $\sim$5–50-nm blocks High angle misorientation of blocks 5°–10°; $\rho = 10^{16}\ \text{m}^{-2}$ Highly dispersed surface layer fractions of μm thick; $\rho = 10^{16}\ \text{m}^{-2}$	Microcrack formation (characteristic size of 10 nm in diameter and 0.1 μm in length) near clusters of deformation defects in slip bands, at grain boundaries and twins Coalescence of nonequilibrium vacancies into submicropores in submicron thickness surface layers Coalescence of submicropores into micropores Surface shearing and delamination regions	Time-localized delamination of a very thin dispersed layer (fractions of μm thick) Petal mechanism Corresponds to high-frequency oscillation of wear intensity and density of deformation defects in time. Hardening and fracture period is $t = 18\times10^3$ s

Table 3. Multiscale selective wear mechanisms (meso and macro)

Structural scales of plastic deformation and failure					
Meso			Macro		
Deformation	Fracture	Wear	Deformation	Fracture	Wear
Growing density of deformation defects in the uncovered layer; $\rho \approx 5\times10^{16}\ \text{m}^{-2}$ Formation of lattice curvature/torsion elements under the action of rotational modes from the overlying deformed layer	Micropore coalescence along boundaries of banded substructure into mesocracks of width 0.2 μm and length $\sim$1 μm (source of quasi-brittle delamination) Fatigue cracking and local cleavage fracture along boundaries of substructural regions (transgranular fracture)	Intensive cracking of subsurface layers and wear debris formation (due to brittle failure) Corresponds to gradual defect density growth in underlying layers with high-frequency oscillation of wear intensity and density of deformation defects in time in the first test stage	Formation of gradient highly porous deformation structure to a depth of a few tens of μm	Micropore coalescence into macropores Mesocrack growth due to plastic deformation and their coalescence into main macrocracks Main (macro) crack formation	Periodic catastrophic wear. Time to this state from the starting point of friction $t = (108\div110)\times10^3$ s at $p = 84$ kPa, $v = 0.45$ m/s in the medium of TsIATIM-201; "layer-by-layer catastrophic selective mechanism" Corresponds to high- and low-frequency oscillation of wear intensity and density of deformation defects in time. Reduction of high-frequency oscillation period from 18.0×10^3 s to 2.3×10^3 s. Low-frequency oscillation period is $\approx(25\div26)\times10^3$ s

multiscaling. This determines a wide size range of wear debris and their tendency to refine with time.

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