MESOSCOPIC LEVELS OF PLASTIC FLOW WITHIN SURFACE LAYERS OF POLYCRYSTALS AND THEIR FATIGUE FRACTURE UNDER CYCLIC BENDING

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ABSTRACT

It is shown that within the surface layers of titanium, aluminum, lead and lead base alloy polycrystals under alternating bending there forms multilevel mesosubstructure, which governs the nucleation of surface fatigue cracks. The type of mesosubstructure and the size of structure elements are determined by the shear stability of surface layer internal structure as well as by the elastic characteristics of the substrate. The discussion is based on the theory of localized inelastic deformation waves.

1. INTRODUCTION

In the framework of physical mesomechanics basic concept a deforming solid is regarded as a multilevel system in which plastic flow evolves on three scale levels, i.e. micro-, meso- and macroscopic ones [1]. A deforming polycrystal's surface layer is an autonomous mesoscopic structural level on which mesoscopic mechanisms of plastic flow would occur much more readily than within the material bulk.

By the active loading of polycrystals at room temperature, the deformation occurs mainly by dislocation motion on the micro-scale level. All the processes responsible for the deformation on the higher-lying meso-scale level occur in concurrence with the deformation, which involves dislocation motion on the micro-scale level. This hampers the development and manifestation of the underlying deformation mechanisms occurring on the mesoscopic structural levels.

Mesoscopic deformation mechanisms are expected to occur intensively at room temperature within polycrystals' surface layers during cyclic loading below the macroscopic yield limit. Low mechanical characteristics of the polycrystal's surface layer are related to its structure specific features [2, 3], which enables the material within this layer to deform even if the material bulk is loaded well below the yield limit [4]. The elastically deformed "substrate" causes loading of the plastically deforming surface layer according to cyclic compression-tension scheme. Conjugation of the substrate and of the surface layer causes the effect of corrugated surface layer. Stress concentrators form in local curvature zones. Relaxation of the stress concentrators involving generation of dislocations into the elastically deforming "substrate" is hampered; therefore, an increase in the number of loading cycles would cause the number of stress concentrators in the surface layer to grow continuously. As a consequence, the excess of deformation defects in the surface layer of the specimen under cyclic loading will increase continuously so that the density of defects exceeds by one or two orders that of the material bulk [5, 6]. This favors involvement into the process of plastic flow of the mesoscopic structural levels.

It stands to reason that the evolutionary behavior of deformation within polycrystals' surface layers is determined by a number of factors, i.e. surface layer structure and phase state, extent of grain-boundary sliding (GBS), shear stability of crystal lattice and of surface layer internal structure.

The present paper presents the results of investigation of the regular features exhibited by deformation and fatigue fracture on the mesoscopic structural levels within the surface layers of

metal and alloy polycrystals, which differ with respect to the extent of grain-boundary sliding and shear stability of their internal structure. The materials were tested in alternating bending at room temperature.

2. MATERIALS AND EXPERIMENTAL METHODS

The investigation was performed using polycrystals of titanium, aluminum, lead and lead base alloys. These metals differ with respect to their melting points. Aluminum and lead are monomorphic metals with FCC crystal lattice. Of fundamental importance is the difference in the shear stability of metals' internal structure. The shear stability of a polycrystal's internal structure can be evaluated qualitatively from the shear modulus G, stacking fault energy γ , and extent of GBS.

Thus lead has relatively low G and γ values and high extent of GBS. Alloying elements for lead are chosen so as to cause changes in its grain–boundary state and in the crystal lattice within the grain volume, thereby varying the kind of dynamic mesosubstructure that forms in the material under cyclic loading. Aluminum has high stacking fault energy and high shear stability of its internal structure; at 293 K in this material no GBS is found to occur. Titanium has a very high melting point and very low stacking fault energy; in this material twinning is liable to occur readily. Titanium differs from lead and aluminum with respect to crystal lattice type (*a*-Ti has HCP lattice); besides, titanium is a polymorphic metal. Titanium also has high values of G and T_{melt} .

The tests were conducted using flat specimens whose gauge length was 40 mm and whose crosssection was $8x1 \text{ mm}^2$. The fatigue tests were performed at room temperature according to alternating console bending scheme at a frequency of 430 min⁻¹. In the case of lead and lead base alloys, the bending amplitude was $\pm 0.5 \text{ mm}$ and in the case of aluminum and titanium, $\pm 1 \text{ and } \pm 3 \text{ mm}$, respectively. A 3D image of the mesosubstructure which forms within the specimen surface layer was obtained with the aid of an *Axiovert-25 CA* microscope equipped with a DIC unit designed for achieving differential-interference contrast.

3. RESULTS OF INVESTIGATION

On the base of the theory of vortex mechanical field in a deforming solid [7] a synergetic criterion of plasticity is formulated in [8] as equality of the curls of primary glide and of accommodation secondary fluxes of all kinds of deformation defects

$$(\operatorname{Rot}S^{a\mu}) = V(\operatorname{Rot}R^{a})^{\mu} \tag{1}$$

where V is the rate of overall deformation $d\epsilon/dt$.

The physical meaning of (1) is interpreted as follows. One can single out from a deforming material certain volume within which the net vortex of deformation defect fluxes is equal to zero:

$$\sum_{k} \operatorname{Rot} J_{k} = 0 \tag{2}$$

where J_k is the *kth* flux of deformation defects. The above volume has linear size l, which characterizes the higher-lying structural level of deformation one has to take into account by addressing a deforming solid viewed as a multilevel system. The structural investigations have yielded evidence which supports the above statement. Thus it has been shown that, depending on the shear stability of the polycrystal's internal structure, in the material tested in alternating bending there forms mesosubstructure-II. The mesosubstructure-II is characterized by parameter l whose value is intermediate between the average grain size of the material and the specimen cross-section. The kind of mesosubstructure-II, which forms within the surface layer of the polycrystal at

the first stage of cyclic bending, determines the subsequent fatigue fracture of the material. In what follows the results obtained for the materials investigated are considered.

Lead and lead base alloys. Lead polycrystals have low shear stability of its internal structure. Lead specimens have high value of $T_{\text{test}}/T_{\text{melt}}$; therefore, the formation of mesoscale level of deformation in this material is especially well pronounced. Thus localized deformation mesobands are found to develop in the conjugate directions of maximal tangential stresses, τ_{max} , passing through a number of grains. Upon mesoband overlapping, there forms mesosubstructure-II, which consists of blocks, each block incorporating several grains or grain fragments of the original polycrystal.

The underlying mechanism responsible for the formation of the above mesosubstructure is one of single slip, which occurs within the grains with a concurrent rotation of the same grains as units. It initiates intensive GBS on the grain boundaries. Due to constrained GBS, on the location of grain-boundary curvature there emerges local stress concentrator. As the number of loading cycles increases, disclination is generated in the above zone, which causes the mesoband of localized translation-rotation deformation to extend within a grain in the direction τ_{max} .



Figure 1: The large-scale rectangular mesosubstructure-II in the lead specimen surface layer, $N = 5 \times 10^3$ cycles; \times

The mesobands extending in the conjugate directions τ_{max} through a number of grains would undergo self-organization, which causes rectangular mesosubstructure-II to form in the surface material layer (Fig. 1). In point of fact, large-scale fragmentation is taking place in the deforming polycrystal. As soon as the formation of mesosubstructure-II is completed over the entire width of the specimen surface, further accommodation restructuring occurs in the polycrystal, which involves enhancement of the rotation processes within the above bands. Eventually, at a comparatively small number of loading cycles, this brings about fatigue crack initiation and propagation along mesobands. Lead base alloy was obtained using an appropriately chosen addition. The resultant lead base alloy has enhanced shear stability. It is found that GBS in the surface layer of as-obtained alloy is hampered, that precludes formation of adverse rectangular mesosubstructure-II and increases significantly the life time of the material under cyclic loading. If alloying of lead causes a decrease of the shear stability of its internal structure, its life time is reduced considerably.

Aluminum. Aluminum exhibits high shear stability of its internal structure and considerably long life time by cyclic loading. Thus alloying of lead was carried on using tellurium as alloying addition. As-obtained alloy has enhanced shear stability and its life time is 2.5 times that of the original material (the life time of aluminum is 1.5 times that of lead).

In fine-grained aluminum specimens under cyclic loading there forms mesosubstructure-II, which consists of conglomerates of self-consistently deforming grains (Fig. 2). Aluminum and tellurious lead have about equal original grain size (70 μ m). When specimens of these materials are tested in alternating bending, in their surface layers there form similar mesoscopic substructures, which have the form of loops. However, mesosubstructure development in aluminum surface layer takes a considerably larger number of loading cycles relative to lead base alloys.

The above experimental evidence supports the validity of Eqs. (1) and (2). In accordance with (1) and (2), one can single out in the deforming material certain volumes within which the net vortex





Figure 2: The mesosubstructure-II in the aluminum specimen surface. N = 5×10^6 cycles. Designated by numbers are the self-consistently deforming grains within the conglomerates; $\times 100$

Figure 3: The surface structure of the recrystallized VT1-0 titanium specimen, $N = 20 \times 10^6$ cycles; x500

of deformation defect fluxes is equal to zero. In the material under cyclic loading there form closed conglomerates of self-consistently deforming grains, which now begin to play the role of structural element of deformation (instead of the original grains). Thus structural elements grow dramatically in size with a concurrent significant increase in the level of stress mesoconcentrators on their boundaries. At the first stage relaxation of the mesoconcentrators involves material fragmentation within the closed conglomerates of self-consistently deforming grains. Upon further loading of the specimen, rotation of material fragments is enhanced. When the imposed strains are no longer accommodated by fragmentation with concurrent fragment rotation, another relaxation mechanism begins acting, i.e. cracking is initiated, which leads to material fatigue fracture.

Commercial-grade titanium. A comprehensive study of mesosubstructure, which forms within surface layers, has been made using VT1-0-grade titanium specimens tested in alternating bending. The material internal structure is found to exhibit anomalously low shear stability. On the recrystallized titanium specimen surface tested in alternating bending there is observed multilevel mesosubstructure formation. This involves surface layer corrugation, motion of grains as a unit with concurrent GBS and self-organization of extruded grains into loop-shaped conglomerates within which intrusion of surface grains takes place.

Ultrasound treatment and saturation with hydrogen of the titanium specimens' surface layers enhances dramatically the effect of surface mesosubstructure. As is seen from Fig. 3, the grains move as units and the extruded grains deform in a self-consistent fashion to give loop-shaped conglomerates with loops 40 - 60 μ m in diameter. Analogous loops observed in aluminum and Pb+0.3%Te surface layers have diameters, respectively, four and ten times that of the titanium specimens. The shear modulus values for the above materials are approximately in the same reverse ratio of 1:4:10, respectively. The above correlation appears to be a logical one since formation of loop-shaped mesosubstructure is due to the plastically deformed grains within the surface layer being conjugated with the elastically deformed substrate. It is the substrate which provides for the fulfillment of condition (2).

Figure 4a shows the surface roughness of the titanium specimen illustrated in Fig. 3 as well as the corresponding cross profile of a portion of its surface. As is seen from Fig.4a, the specimen surface has a corrugated profile with wavelength of $\sim 150 \ \mu\text{m}$ and fold height of $\sim 0.4 \ \mu\text{m}$. Thus the modulation of the polycrystal surface profile is comparable to its average grain size. As a result of ultrasound treatment, nanostructure is found to form in the material surface layer. As-treated material specimens tested in alternating bending are found to reveal no surface profile modulation (Fig. 4b).



Figure 4: The surface roughness and the corresponding cross profile of the recrystallized titanium specimen tested in alternating bending: coarse-grained surface, $N = 20x10^6$ cycles (a); nanostructured surface layer, $N = 14.5x10^6$ cycles (b); ×500

As a result of saturation of titanium surface layers with hydrogen, the material behavior by active tension is found to change significantly. The presence of hydrogen is discovered in as-received VT1-0 titanium, which might favor the formation of surface mesosubstructure during the cyclic loading of the material. Therefore, a special saturation of titanium surface layer with hydrogen has been performed. As-treated titanium surface layer reveals the occurrence of mesosubstructure comprising grain conglomerates. The subsequent testing of the titanium specimens by alternating bending causes a strongly pronounced effect of extrusion-intrusion of the above grain conglomerates within the material surface layer. Characteristically, in the extruded grain conglomerates there develops single slip, which is not inherent in crystalline materials.

The conjugation of the plastically deformed grain conglomerates within the surface layers with the elastically deformed substrate brings about mesosubstructure formation on the higher-lying mesoscale level-II. The mesosubstructure comprises closed superloops of extruded grain conglomerates. The average size of superloops is ~ 200 μ m; the average difference in height for extruded and intruded grain conglomerates within a superloop is ~ 1.5 μ m. Superloops are located in the transverse band of the specimen where the bending amplitude reaches a maximal value. Therefore, it is in this band that the main crack of fatigue failure is initiated at the final stage. However titanium has higher strength of bonding in the crystal lattice and hence higher fatigue strength relative to aluminum.

4. DISCUSSION OF RESULTS

The above regular features of mesosubstructure formation in the polycrystals' surface layers are associated exclusively with the effect of multiscaling exhibited by the surface layer-substrate system. As metallic polycrystals are being tested in alternating bending, residual plastic strains accumulate in their surface layers. The plastically deformed surface layer is conjugated with the elastically deformed substrate, which results in the formation of residual corrugated surface layer. Thus, consideration of the mechanisms involved in the deformation of materials tested in alternating bending should necessarily include the virtual interface "plastically deformed surface layer/elastically deformed substrate".

No adequate theory has been developed thus far in order to address similar multiscale processes, which occur in the surface layers of deforming solids. However, some of the mechanisms responsible for the deformation on the mesoscale level are described fairly well in [1, 9].

The theory [1, 9] predicts the vertical motion component for deforming grains or grain conglomerates in the deforming material surface layer. This also gives an adequate description of the formation of block structure in the surface layer of coarse-grained lead specimens tested in alternating bending (Fig.1). In this instance, material rotation involving intragranular single slip results in local grain-boundary curvature. Along the grain boundaries there moves a soliton of form-changing as non-linear grain-boundary sliding wave. The motion of GBS soliton is accompanied by surface grain rotation behind of the soliton front. Due to the interaction of the surface grain with the elastically deformed substrate, reversal rotation of the surface grain there emerges disorientation boundary in the form of a kink band, which causes its reversal rotation behind the soliton front. This process brings about relaxation of internal stresses, which build up on the interface between the elastically deformed substrate and a portion of the surface grain in which grain-boundary sliding has occurred. Disoriented substructure development occurring in the surface layers of coarse-grained lead specimens tested in alternating bending ends in fatigue failure of the material.

The rotation modes of deformation, which are associated with the motion within the surface mesosubstructure loops of nonlinear localized plastic flow wave, bring about fatigue crack initiation in side loop volumes. These modes are also associated with the incompatibility of loop rotation, which involves plastically deformed grains and the elastically deformed substrate. In this connection it is pertinent to mention that good correlation exists between the size of blocks/mesosubstructure loops and the shear modulus of the substrate material.

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