MULTILEVEL WAVE MODEL IN FRACTURE MESOMECHANICS

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ABSTRACT

Relying on the analysis of the author and his co-worker's data, this overview substantiates the basic propositions of the multilevel wave model in fracture mesomechanics. Any solid under loading is considered as a self-organized multilevel system where plastic flow and fracture are two subsequent stages of shear-stability loss at the micro-, meso- and macroscale levels. Fracture is global shear-stability loss in a loaded specimen. Two parallel (in the shape of a dipole) or conjugate (in the shape of a cross) macrobands of plastic flow localization propagate throughout the specimen cross section. They evolve self-consistently by the "phase wave" mechanism. The macrobands are characterized by strongly localized material rotation, which is accompanied by mesofragmentation of the surrounding material as the accommodation mechanism of rotation. For macrobands conjugated in the shape of a cross there are two kinds of their self-consistency. At the first stage, the self-consistency between two half-macrobands at each side of the specimen takes place. The rotation modes of the two coupled half-macrobands are accommodated by mesofragmentation of the surrounding material. It is accompanied by the formation of a ductile neck. At the definite extent of mesofragmentation the accommodation ability of the deformed material within the area of coupled macrobands is exhausted. Then the self-consistency between the coupled half-macrobands at each side of the specimen breaks down and the neck formation is stopped. At the second stage of loading, there arises the self-consistency between half-macrobands from the opposite sides of the specimen. It is accompanied by crack propagation throughout the cross section and causes fracture of the loaded specimen. For the dipole configuration of the two opposite macrobands their self-consistency across the entire cross section arises from the very beginning. It results in quasi-brittle fracture of the specimen. The prefracture criterion of a solid under loading based on a multilevel wave model is discussed.

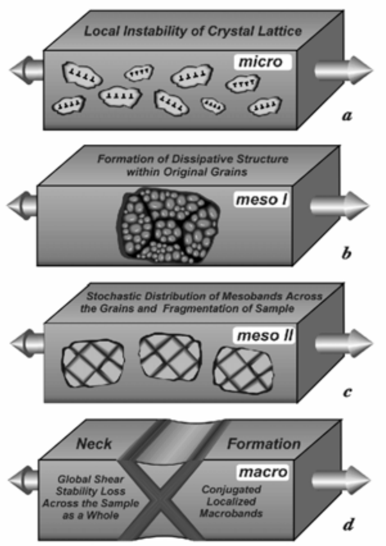

Figure 1: Schematic representation of scale levels of shear stability loss in deformed solid: micro (*a*); meso I (*b*), meso II (*c*), macro (*d*)

1. INTRODUCTION

Plastic deformation and fracture of a loaded solid are associated with the loss of its shear stability and evolve as a multilevel relaxation process [1,2].

Initially, the loss of shear stability takes place at the microlevel in localized zones of the crystal lattice. Stress microconcentrators (SMC) formed at structural heterogeneities cause local rearrangement of the crystal lattice in specific crystallographic directions. These local structural transformations are manifested in the initiation and motion of dislocations as fragments of another crystal lattice, Fig. 1(*a*). The effect of SMC is entirely of the short-range type and, consequently, the dislocations travel over small distances only in the zone of SMC. It is assumed that individual dislocations are translational defects and provide only translational strain modes.

The crystallographic character of the dislocation motion that does not coincide with the axis of loading necessitates the self-organization of dislocation ensembles according to given boundary conditions (the specimen axis must remain unchanged). As a consequence, the dislocation ensembles form dissipative substructures within the original internal structure of a specimen, Fig. 1(*b*). Such dissipative substructures provide vortex plastic flow according to the scheme "shear + rotation" and are classified in [1,2] as mesoscale level I.

At deformation the density of dislocations (and of other defects) increases and when a particular critical value is reached, the loss of shear stability occurs in local areas of a specimen as a unit. Structural rearrangements may take place over large distances and in arbitrary directions but not only in crystallographic ones. This scale level of shear stability loss is classified in [1,2] as mesolevel II. New types of defects appear at mesolevel II, viz. mesodefects: such as disclinations and banded structures of different types (microbands, microtwins, martensite plates, etc.), Fig. 1(*c*). They form in the vicinity of stress mesoconcentrators (SMEC) and propagate over large distances through a great number the structural elements, irrespective of their crystallographic orientation. Mesodefects contain both shear and rotational strain components. They cause three-dimensional mesovolumes of different mesoscales (subgrains, grains, their conglomerates, elongated blocks of material) to move within a solid under deformation.

Finally, localized macrostress concentrator s develops in a deformed solid which gives rise to two parallel or conjugate macrobands penetrating through the entire cross-section of the specimen, Figs. 1(*d*) . It is global loss of shear stability of a deformed specimen which manifests itself as neck formation and a drop in the applied stress. The corresponding stage of the descending stress-strain curve must be considered as the fifth stage of plastic flow in addition to four stages of plastic flow in common use.

A great deal of fracture types is related to different self-organization of shear stability loss scale levels. Let us consider the main propositions of multilevel wave model in fracture mesomechanics.

2. SURFACE SWITCHING WAVES IN THE MULTILEVEL MODEL OF A SOLID UNDER DEFORMATION

According to the synergetic principles of physical mesomechanics [1], plastic flow of a deformed solid develops as the superposition of wave processes of its shear stability loss at different structural levels. Each structural level of plastic flow is associated with its corresponding scale level of stress concentrators. A base stress concentrator emerges at the point at which an external load is applied to a deformed solid. This stress concentrator generates all primary shears. The evolution of the latter in the hierarchy of structural levels of deformation depends on the initial internal structure of a material and on the conditions of its loading.

In the general case, the primary non–linear waves of plastic flow propagates from the base stress concentrator in thin surface layers of a material, which are characterized by a low shear stability, by an extremely high vacancy density, and by the presence of a wide range of atomic configurations [5–7]. In terms of synergetics, these waves are called surface switching waves.

The flow of surface defects is initiated near a movable grip, propagating in the direction of maximum tangential stresses τ_{max}. The crystalline substrate is therewith deformed elastically, thereby retarding the evolution of the flow of surface defects. In the surface layer, a fold with a clearly defined curvature is formed in which microstress concentrators arise. This fold is a place where primary dislocations responsible for plastic flow of a material are generated going to the material bulk within the field of the microstress concentrator gradient [8]. The front of surface shears propagates further, generating new dislocation chains. The deformation localization of this kind covers the submicron range.

Should one retard the generation of dislocations in the submicron range by specially choosing a material, the formation of macrobands of localized deformation in surface layers may then be observed in the millimeter range [9,10].

The primary plastic shears, which propagate in a surface layer of the specimen in the direction of τ_{max} arise near one of the movable grips. The front of these shears advances along the deformed specimen, causing its bending and transverse deflection from the specified loading axis. As a result, kink bands in the form of macrobands of localized deformation make their quasiperiodic appearance parallel to the front of primary shears. The distance between adjacent kink bands is 1–2 mm. When a kink band is generated, there is a jump on the "stress – strain" curve.

As the front of primary surface shears approaches the second movable grip, it is then reflected from the specimen end, propagating in the opposite direction. The vectors of surface displacements therewith change their direction to the conjugate one $\overline{\tau}_{max}$ and the transverse deflection of the specimen reverse its direction. When repeatedly reciprocating along the loading axis, the front of primary surface shears causes the specimen to self-oscillate transversely, much like a violin string does. The bands of localized deformation emerging in the process engulf successively the entire specimen volume, thereby executing its plastic flow in a purely local manner. In synergetics, such a process is classified as the motion of a traveling pulse in an excited medium.

The character of the kink bands produced by the moving front of surface shears depends on the type of a material and on the type and conditions of loading.

3. EVOLUTION OF QUASIHOMOGENEOUS PLASTIC FLOW AND THE FINAL STAGE OF ITS MACROLOCALIZATION

As the dislocation density in a deformed specimen is increased its rigidity increases and the size of the zone where the specimen undergoes active deformation decreases, too [9-11]. The primary and reflected fronts of surface switching waves move farther and farther away from the ends of the specimen gauge section. Such a situation is equivalent to the case wherein the virtual grips of a test machine, which act as base stress concentrators, approach each other.

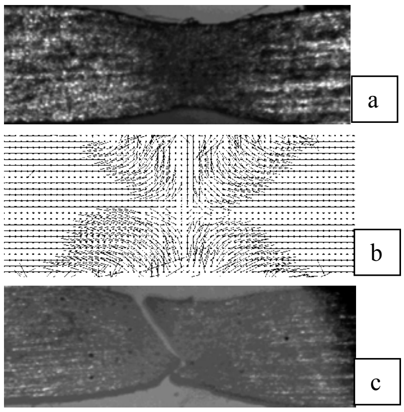

Figure 2: Formation of a neck and the character of fracture of a cold-rolled Ti specimen with a submicrocrystalline surface structure under tension: an optical image of the specimen surface (a); the displacement vector field at the submicrocrystalline surface (b); the character of fracture of the specimen (c); ε = 17 %.×15 [12]

The average velocity of the τ_{max}-oriented front of the primary surface wave propagating along the specimen decreases progressively and an abrupt change in its direction for the conjugate one $\overline{\tau}_{max}$ takes place. In the limiting case, the transversely self-oscillating zone of active deformation decreases to the size of the region where the direct and reflected fronts of surface switching waves are met (or mutually superimposed). In this region, the primary and reflected fronts form either a cross of conjugate macrobands of localized deformation (Fig. 2) or a dipole of opposing parallel shear macrobands (Fig. 3). It is this active zone that determines the place where a neck is formed and a wave process of global shear stability loss of a deformed specimen evolves.

It does not always happen that one can manage to reveal macrobands of localized deformation in the neck in ordinary polycrystalline specimens under tension. The microscale dislocation deformation smears the macrobands, causing them to be weakly pronounced. However, if we retard the dislocation deformation, e.g., by forming a submicrocrystalline structure or a nanostructure at the surface or in the material bulk, the genesis of macrobands and the wave character of their evolution can clearly be defined in the displacement vector field on the descending portion of the "stress – strain" curve.

Two kinds of plastic flow macrolocalization in tensile flat specimens of submicrocrystalline α-Fe are presented in Fig. 4. Very low ductility of such specimens causes fast development of plastic flow macrolocalization by a combination of localized mesobands in parcels. Macrostress concentrators at the ends of the gauge length of a dumbbell-shaped specimen generate either a dipole of opposing parallel shear macrobands (Fig. 6,*a*,*b*,*c*) or a cross of two overlapping macrobands (Fig. 4,*d*,*e*,*f*). The rest of the specimen gauge length remains elastically deformed up to fracture. The evolution scheme of both kinds of macrolocalization is shown in Fig. 5.

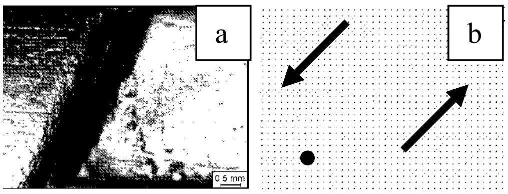

Figure 3: Formation of a dipole of macrobands of localized deformation in the prefracture zone of tensile armco-iron specimen; T = 293 K: an optical image (a); the displacement vector field (b) [16]

As can be seen in Fig. 7,*a* the development of the primary macroband *AB* in the dipole configuration is accompanied by the local material rotation of the specimen. Under given boundary conditions the specimen axis should remain unchanged. This governs the appearance of a secondary stress concentrator on the opposite lateral face of the specimen. It generates the opposing localized deformation macroband *CD* into the specimen bulk. The material rotation associated with the macroband *CD* has an opposite sign as compared to the sign of the material rotation induced by the primary macroband *AB* (Fig. 7,*a*).

This satisfies the given boundary conditions. Fig. 5,*a* also shows decomposition of shear vectors in the primary and secondary macrobands. Their accommodation brings about two important results:

1. The longitudinal shear components in the macrobands induce relative displacements of different specimen parts along the tension axis. Shear in the primary macroband AB gives rise to the displacement by tension of the zones ABLK and ABMN. An opposing shear in the secondary macroband CD gives rise to the displacements by tension of the zones CDKL and CDNM. The narrow zone *ABCD* experiences oscillatory longitudinal motion as a whole adjoining alternately the macroband *AB* and macroband *CD*.

2. The transverse shear components in the macrobands *AB* and *CD* generate a pair of forces acting on the zone *ABCD* between the dipole of opposing macrobands. This governs a crystallographic rotation of the zone *ABCD*, which steadily increases with strain growth. This process is accomplished by crack propagation along one of the two dipole macrobands causing quasibrittle fracture of the tensile specimen.

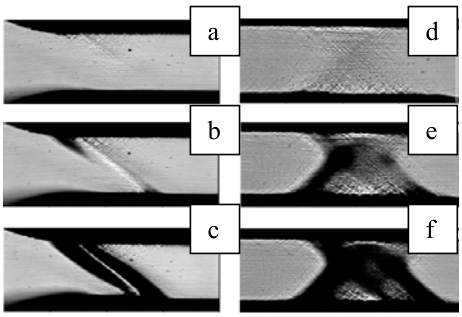

Figure 4: Different types of propagation of localized deformation meso- and macrobands: ε = 3 (a, d), 4 (b, e) and 5 % (c, f). Image size: 5.7 × 2.6 mm^2

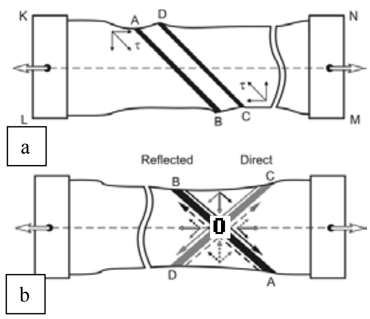

Figure 5: Schematic representation of shear accommodation in interaction of localized deformation macrobands in the form of a dipole (a) and a cross (b)

The case of the self-consistent development of mesobands by the scheme of a cross of self-conjugate macrobands is shown in Fig. 5,*b*. The specimen elongates mainly due to deformation inside the macrobands. In the bulk of the trihedral prisms *AOD* and *BOC* between intersecting localized deformation macrobands displacement vectors are directed into the specimen (Fig. 5,*b*). That is why the trihedral prisms are material fragments indented into the bulk of the tensile specimen. Such a scheme of stress-strain state corresponds to tension in the conditions of local lateral pressure. This favors local plasticity and neck formation. The width of the zone of a macroband cross increases with strain growth. The development of the macrobands through the whole specimen cross-section governs a global loss of shear stability and formation of a localized neck in the specimen.

For macrobands conjugate in the shape of a cross there are two kinds of their self consistency. At the first stage, the self-consistency between two half-macrobands at each side of the specimen takes place. The rotation modes of the two coupled half-macrobands are accommodated by meso-fragmentation of the surrounding material. It is accompanied by the formation of a ductile neck. At the definite extent of meso-fragmentation the accommodation ability of the deformed material within the area of coupled macrobands is exhausted. Then the self-consistency between the coupled half-macrobands at each side of the specimen breaks down and the neck formation stops. At the second stage of loading, there arises the self-consistency between half-macrobands from the opposite sides of the specimen. It is accompanied by crack propagation throughout the cross section and causes fracture of the loaded specimen. For the dipole configuration of the two opposite macrobands their self-consistency across the entire cross section arises from the very beginning. It results in quasi-brittle fracture of the specimen.

The mesomechanics of the prefracture stage for materials in tension and compression is in principle the same. Fig. 6 demonstrates the dipole mechanism of self-organization of localized deformation macrobands at the prefracture stage for a compressed specimen from composite Cu–TiB_2. The disperse hardening by TiB_2 nanoparticles locked the crystallographic sliding of dislocations at the microscale level. The high porosity (~ 15%) governed a low shear stability of the compressed specimen at the meso- and macroscale levels. This caused a rapid development of multiple mesoshears in conjugate directions of τ_{max}.

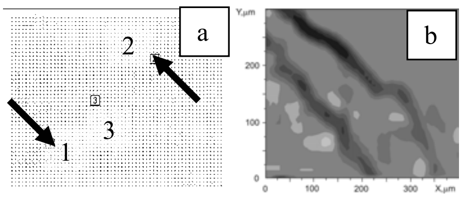

Figure 6: Displacement vector field (a) and rotational component of the distortion tensor (b) in the Cu + 10 % TiB_2 specimen in compression; ε ~ 18.5 %.

The primary macroband of localized plastic shear was generated at $\varepsilon^p = 17.5$ %. It determines a strong material rotation accompanied by the appearance of an extended crack in the macroband.

At the prefracture stage ($\varepsilon^p = 18.5$ %) a strong material rotation in the primary macroband caused generation of an opposing macroband with the material rotation of an opposite sign (Fig. 6,*b*). However, in zone *3* between the macrobands (Fig. 6,*a*) a very strong crystallographic rotation takes place, which ends in quasibrittle fracture of the specimen by the cleavage mode. The main crack propagates along one of the localized deformation macrobands. The specimen is divided into two parts along the direction of τ_{max} in a quasibrittle manner.

The commonness of the prefracture behavior of the material in both tension and compression allows one to state the prefracture criterion: a global shear stability loss in any solid under plastic deformation is related to the development of two macrobands self-organized in the form of either a dipole or a cross in the specimen cross-section. Fracture is the final stage of this process taking place when all accommodation mechanisms at the micro- and mesolevels become exhausted.

4. THE BASIC PRINCIPLES OF A MULTILEVEL MODEL IN PHYSICAL MESOMECHANICS [10]

A multilevel model of a solid under deformation should be conceptually developed according to the following algorithm:

– description of nonlinear waves of plastic flow in the surface layer;
– generation of dislocations at the “nonlinear surface layer – linear crystalline substrate” interface;
– defect generation on internal interfaces;
– formation and development of localized deformation mesobands in the nonlinear medium at the mesoscale level;
– account for the rotational deformation modes at the mesoscale level and evaluation of their contribution to strain hardening of the material;

– nucleation and propagation of cracks at the mesoscale level as noncompensation of opposite-sign rotations;
– mesomechanics of deformation macrolocalization and fracture development as noncompensation of rotations in the macrobands of localized plastic flow.

Clearly that the mathematical development of a multilevel model of a deformed solid will take many years. However, individual blocks of the model will find practical use in the immediate future already.

By way of example let us consider an account for changes in the internal structure of a solid under deformation in the framework of the multilevel model put forward in [12].

Structural state parameters are introduced based on the continuum theory of defects [12] in the form of the defect density tensor and defect flux density tensor [13].

The total deformation of a loaded solid is represented as superposition of:
– compatible elastic deformation due to external action ($\varepsilon^{el, ex}$);
– compatible plastic deformation ($\varepsilon^{pl, c}$);
– plastic ($\varepsilon^{pl, d}$) and elastic ($\varepsilon^{el, d}$) deformation caused by defects.

The compatibility condition implies that material continuity is retained. Compatible plastic deformation governs irreversible changes in the form and makes no contribution to internal stresses. Compatible elastic deformation due to external action is reversible. The sum of elastic and plastic deformations caused by defects meets the compatibility condition, but individually the deformations fail to satisfy this condition. Elastic deformation caused by defects governs internal residual stresses.

To determine translational defects the distortion tensor is introduced. The symmetrical part of the tensor is the deformation tensor. Each structural level of deformation can be represented as a disoriented substructure, which is a scale invariant in the hierarchy of all fragmentation scales for a deformed solid [21]. Each element of the *i*-th substructure is characterized by one plastic distortion varying from element to element.

The principles considered are the basis for the field theory of defects in the multilevel model of a solid under deformation.

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