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PROBLEMS OF MECHANICS OF METAL SURFACE LAYERS

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Mechanics of metal surface layers deals with a description of the following objects, quantities and processes: structures and mechanical properties of metal surface layers after a heat, chemical, electro-chemical or physical treatment; evolution of these structures and properties during mechanical treatments; mechanical behaviour of the layers during exploitation processes. This branch of mechanics is based on the results of physical investigations, but it uses a mechanical approach. In the paper, descriptions of metal surface layers within the classical anisotropic plasticity, large strain plasticity, and finally, the crystal and polycrystal plasticity are recalled. Problems connected with a formulation of laws governing a surface layer behaviour are comprehensively discussed.

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1. Introduction

Mechanics of metal surface layers fringes upon the physics of solids, on one hand, and upon the solid mechanics, on the other. The first deals with a crystal surface and interface properties of the depth scale of $\approx 10^{-6}$ mm, the second describes a mechanical behaviour of metal surface layers of thickness 0.05–5.0 mm. Technological surface layers are composed of various crystal grains, which are stressed, disordered and impure. Their exact mechanical description should take into account the above diversity, but it should remain within the framework of continuum mechanics. Such an approach permits to use many very efficient methods of numerical analysis for a simulation of complex material behaviour. This analysis is based on a system of equations, which determine a current state of a deformed material body. Among these equations, the constitutive laws are particularly important. They are different for different materials (elastic, plastic, viscous, etc.) and they describe behaviour of a small material element. In the case of metals this behaviour is mostly elastic or elasto-plastic. The elastic behaviour is determined by the generalised Hook law. The plastic state and its evolution are defined by a piece-linear or non-linear algebraic equation, known as the plasticity condition, and by the flow rule, which links plastic strain increments with corresponding stresses [1]. In general case, the flow rule contains the fourth order tensor of plastic anisotropy. For metals, the elastic strains are usually small, but the plastic ones may be very large. The plasticity theory at large plastic strains is well elaborated [2], but it is valid for the plastically isotropic materials only. For a correct formulation of anisotropic plasticity at large strain, a microstructure of deformed material must be taken into account [3]. That is why a great progress of crystal and polycrystal plasticity is observed recently [4]. Polycrystalline structure of metal surface layers and their strongly anisotropic properties make it necessary to use the most advanced mechanical models to describe their formation and real behaviour. All these models are based on the notions of the yield stress and hardening moduli. The initial and current yield stress, as well as the initial and current hardening moduli are the basic parameters defining the plastic behaviour of metals. In the classical plasticity, they describe materials without microstructure and they are measured with help of macroscopic specimens. These parameters may be related to micro-hardness of the material, on the microscopic level, or to dislocation densities, on the sub-microscopic level. An identification of the yield stresses and hardening moduli for materials with microstructure is a basic problem of the mechanics of metal surface layer.

2. Structure and mechanical properties of metal surface layers

According to the standard definition, the metal surface layer is a part of a metal element lying under its external surface, which has mechanical, physical and sometimes chemical properties different from those of the core of the element. From mechanical point of view, a surface layer is characterised by a strong plastic anisotropy and a concentration of residual stresses. They appear when the metal element is subjected to one of the following surface technologies [5]:

— heat treatment (e.g. quenching, tempering, annealing),
— chemical treatment (e.g. carbonizing, nitriding),
— electrochemical treatment (e.g. electro-plating),
— physical treatment (e.g. ions implantation).

The plastic anisotropy caused by the above technologies is called the original plastic anisotropy [6]. To temper the stress concentration and to diminish differences between mechanical properties of the surface layer and those of the core, mechanical treatments (rolling and sliding burnishing, shot-peening) are commonly applied [7]. A squeeze of the material during a mechanical treatment leads to the strain induced plastic anisotropy of the layer. Note that the strain induced plastic anisotropy appears also in exploitation processes.

From the mechanical point of view, the most important characteristics determining a state of surface layer are: a structure of the layer, a hardness field and a residual stress field. Examples of these characteristics for a nitrized layer are shown in Fig. 1.

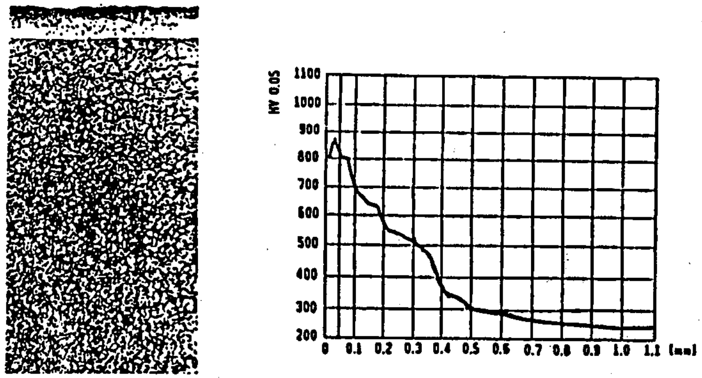

Fig. 1. Structure and corresponding hardness distribution for nitrized surface layer [6].

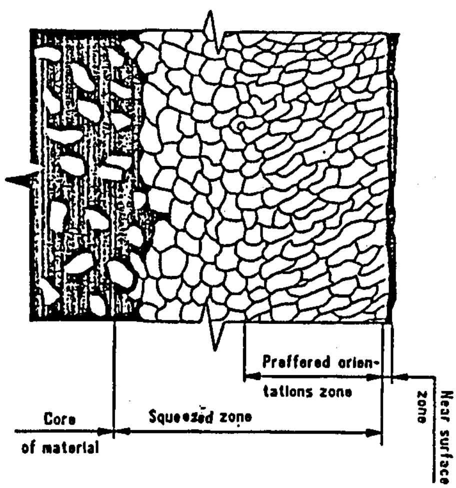

Fig. 2. Structure of metal surface layer according to Polish Standards: *Surface layer. Terminology*, PN 87/M-04 250.

A simplified model of the layer structure is shown in Fig. 2. One can distinguish in the model: a near-surface zone, a preferred surface zone and squeezed zone [8]. Hardening of metal surface layers has strong influence on the plastic localization, and then on localization and initiation of fatigue crack growth in metal elements. Due to high fracture toughness of the surface layers, sources of fatigue cracks are localized under these layers. Many microscopic observations indicate two reasons for appearance and evolution of the strain induced plastic anisotropy [9]:

— an elongation of metallic grains leading to the morphological texture;

— a reorientation of crystalline lattices leading to the crystallographical texture.

The texture effects have a strong influence on the macroscopic properties of metal surface layers. For this reason, mechanical models of layer behaviour should take into account the macroscopic description of metal plastic deformations as well as the microscopic one.

3. Elasto-plastic models of metal surface layers

Thickness of metal surface layer takes values from 0.05 to 5.0 mm. Typical grain diameter is of order of 0.1 mm. Cross-sections of thick surface layers slit so many grains that mechanical properties of the layers may be considered as smoothly changing fields. A principal problem is a way of their determination. In the classical solid mechanics, a material behaviour is tested in uniaxial tension-compression tests and described by stress–strain relations σ–ε. In the case of surface layers, it is better to use intensities of the above tensors for description of their behaviour

$$\overline{\sigma} = \sqrt{(3/2)\sigma_{ij}\sigma_{ij}} \qquad \text{and} \qquad \overline{\varepsilon} = \int_0^{\varepsilon_{ij}} \sqrt{(3/2)\mathrm{d}\varepsilon_{ij}\mathrm{d}\varepsilon_{ij}}. \tag{1}$$

Denote by σ_{ij}, ε^{e}_{ij}, ε^{p}_{ij} and ε_{ij}, the stress, elastic strain, plastic strain and the total strain tensor, and by $\mathrm{d}\varepsilon^{e}_{ij}$, $\mathrm{d}\varepsilon^{p}_{ij}$ and $\mathrm{d}\varepsilon_{ij}$, the corresponding strain increments. Within the small strain considerations one can assume

$$\mathrm{d}\varepsilon_{ij} = \mathrm{d}\varepsilon^{e}_{ij} + \mathrm{d}\varepsilon^{p}_{ij} \qquad \text{and} \qquad \mathrm{d}\overline{\varepsilon} = \mathrm{d}\overline{\varepsilon}^{e} + \mathrm{d}\overline{\varepsilon}^{p}. \tag{2}$$

It may be shown that the relations σ_{ij}–ε^{e}_{ij} and σ_{ij}–ε^{p}_{ij} may be uniquely represented by relations: $\overline{\sigma}$–$\overline{\varepsilon}^{e}$ and $\overline{\sigma}$–$\overline{\varepsilon}^{p}$, respectively [1]. Now, one can introduce a $\overline{\sigma}$–$\overline{\varepsilon}$ relation for a small material element of the surface layer, on the analogy of the σ–ε dependence for standard metal specimens [10] (Fig. 3). This relation depends on the local material parameters: a Young modulus E, an initial yield stress σ_0, a current yield stress σ_y and a current hardening parameter H. In the standard uniaxial tension test, the above quantities are assumed to be constant on the cross-section of metal specimen. Here, these quantities change through the depth

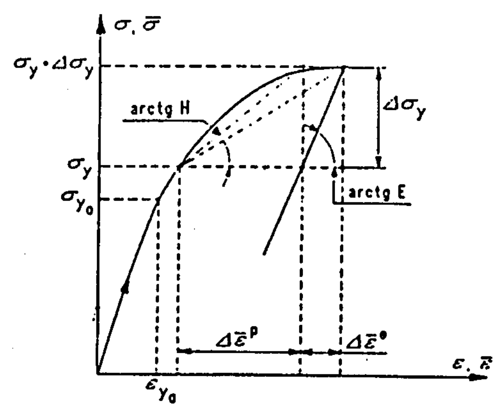

Fig. 3. Stress–strain relation for small material element of metal surface layer.

of the surface layer and their identification makes many problems. Assuming elastic isotropy of the layer, the parameter E is commonly taken the same as that in the core. The identification of σ_0, σ_y and H parameters is more complex. Most often these parameters are determined indirectly, with help of hardness tests [11].

When the stress state is a three-dimensional one, the initial and current yield stresses form, in the principal stress space $\{\sigma_1, \sigma_2, \sigma_3\}$, the initial and current yield surfaces. For metals these surfaces are cylindrical, and their axes are equally inclined to the principal stress axes. During an anisotropic plastic yield of the material element, cross-section of yield surfaces is deformed, and their axis is shifted from the initial position.

Two facts are ascertained and experimentally confirmed:
— yield stress is independent on the hydrostatic pressure $\sigma = \frac{1}{3}\sigma_{ii}$, i.e. it depends on the deviator s_{ij} only;
— plastically deformed material is incompressible one, i.e. $\varepsilon^{\mathrm{p}}_{ii} = 0$.
Taking the above into account, the general form of the quadratic yield surface is the following:

$$F(\sigma_{ij}, \sigma_y) \equiv \frac{1}{2} A_{ijkl}(s_{ij} - \alpha_{ij})(s_{kl} - \alpha_{kl}) - \frac{1}{3}\sigma_y^2 = 0. \tag{3}$$

In the expression (3), $A_{ijkl} = A_{ijkl}(\varepsilon^{\mathrm{p}}_{pq})$ is the fourth order tensor of plastic anisotropy moduli, $\alpha_{ij} = \alpha_{ij}(\varepsilon^{\mathrm{p}}_{pq})$ is the kinematical hardening tensor, and $\sigma_y = \sigma_y(\bar{\varepsilon}^{\mathrm{p}})$ is the current yield stress. An evolution of α_{ij} is governed by an additional hardening rule. The tensor α_{ij} describes a shift of the yield surface axis from the initial position and it is responsible for a difference between the yield stress during a tension and that during compression (i.e. the Baushinger effect).

The most popular approach to description of plastic anisotropy of metals is the orthotropic theory of plasticity proposed by Hill [1]. Within this approach, the yield condition takes the form

$$\begin{aligned} F(\sigma_{ij}, \sigma_y) \equiv F(\sigma_{22} - \sigma_{33})^2 + G(\sigma_{33} - \sigma_{11})^2 + H(\sigma_{11} - \sigma_{22})^2 \\ +2L\sigma_{23}^2 + 2M\sigma_{31}^2 + 2N\sigma_{12}^2 + \frac{2}{3}\sigma_y^2 = 0. \end{aligned} \tag{4}$$

In this yield condition, the Baushinger effect is neglected. The fixed parameters: F, G, H, L, M and N describe an initial anisotropy of the plastic yield. They are determined in the stress–strain tests. A proposition of model which describe changes of plastic anisotropy during a deformation process has been given by Baltov and Sawczuk.

To complete a model of plastic behaviour of the material, it is necessary to postulate the flow rule which expresses a plastic strain rate $\dot{\varepsilon}_{ij}$ through the stress tensor σ_{ij}. For metals, the plastic flow rule is associated with the assumed yield condition

$$\dot{\varepsilon}_{ij} = \dot{\lambda} \frac{\partial F}{\partial \sigma_{ij}}. \tag{5}$$

It means that the function $F(\sigma_{ij}, \sigma_y)$ is a plastic potential for the field $\dot{\varepsilon}_{ij}(\sigma_{ij}, \sigma_y)$. The scalar function $\dot{\lambda} = \dot{\lambda}(\sigma_{ij}, \dot{\sigma}_{ij})$ is determined from the consistency condition

$$\dot{F}(\sigma_{ij}, \sigma_y) = 0. \tag{6}$$

The above condition results from an assumption that the plastic strain rate does not depend on load rates and consequently on a time scale. This assumption makes the fundamental difference between the plastic and viscous material behaviour. Whereas the viscous stress field strongly depends on a deformation rate, the plastic one depends on a load magnitude only.

The relations (4)–(6) enable to construct the rigid-perfectly plastic model of the material neglecting elastic strains and hardening. One can predict properties of squeezed surface layer after the roller burnishing under a high load (Fig. 4). Now,

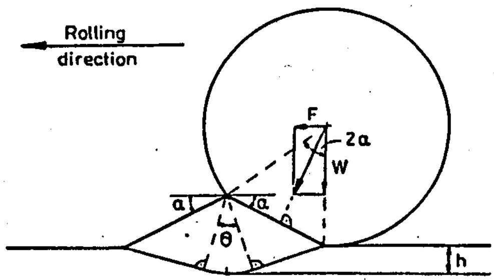

Fig. 4. Plastic zone and squeezed surface layer of rolled material.

let us consider the elasto-plastic model. The elastic strain rate of the material may be determined from the generalized Hook law expressed in the incremental form

$$\dot{\sigma}_{ij} = L_{ijkl}\dot{\varepsilon}^{e}_{kl}, \tag{7}$$

where L_{ijkl} are components of the fourth order tensor of elastic moduli.

From (2), (5) and (7), one can obtain the following Prandtl–Reuss equations:

$$\dot{\sigma}_{ij} = (L_{ijkl} + \kappa C_{ijkl})\dot{\varepsilon}_{kl}, \tag{8}$$

where $C_{ijkl} = C_{ijkl}(s_{pq})$ are components of the fourth order tensor of plastic anisotropy moduli, $\kappa = 0$ for $F(\sigma_{ij}, \sigma_y) < 0$ and $\kappa = 1$ when $F(\sigma_{ij}, \sigma_y) = 0$. The above equations may be directly used in numerical procedures for analysis of metal surface layers. As an example [13], results of residual stress calculations for an elastic-plastic surface layer after rolling a metal element are shown in Fig. 5. On the plot a denotes the roller–element contact width, and p_0 is the maximum contact pressure.

Let us examine the case of large plastic strains, which appear during loading of metal specimen. As it was previously observed, the plastic strain may be defined as that remaining after elastic unloading of the specimen. However, such a definition is correct for uniform strains only. In the case of nonuniform strains, residual distortions remain in the specimen after unloading. To remove them, one can cut the specimen onto small unstressed pieces. The final strain of each of them may be regarded as the plastic strain. The above procedure has been proposed by Lee [2] and it is known as the hypothesis of unstressed configuration. According to this hypothesis, for large plastic strains instead of the additive rule (2), the following multiplicative rule is introduced:

$$F_{ij} = F^{e}_{ik}F^{p}_{kj}, \tag{9}$$

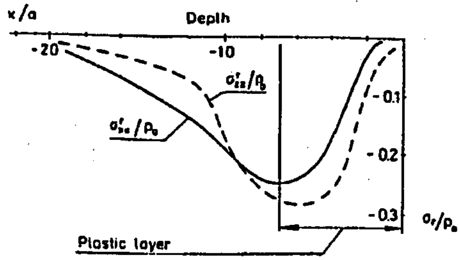

Fig. 5. Residual stresses in metal surface layer after rolling.

where F^{e}_{ik}, F^{p}_{kj} and F_{ij} are the elastic, plastic and the total deformation gradient, respectively.

Note that the final orientations of unstressed pieces of the specimen are not determined. Then, the hypothesis of unstressed configuration is valid providing that the stress–strain relation for each of the pieces does not depend on its orientation. It is the case of isotropic material. For that case, McMeeking and Rice [14] have proposed a generalization of the Prandtl–Reuss equations (8) on the case of large plastic strains. Their form is the same as for small strain theory, but instead of the Cauchy stress rate $\dot{\sigma}_{ij}$, the Jaumann derivative of the Kirchhoff stress

$$\tau^{\nabla}_{ij} = \dot{\tau}_{ij} + \tau_{ik}\omega_{kj} - \omega_{ik}\tau_{kj} \tag{10}$$

is introduced, and on the place of $\dot{\varepsilon}_{ij}$ the strain rate tensor d_{ij} is set down. The quantities τ_{ij}, d_{ij} and ω_{ij} are defined as follows:

$$\tau_{ij} \equiv \frac{\rho}{\rho_0}\sigma_{ij}, \quad d_{ij} \equiv \frac{1}{2}(F_{ij} + F_{ji}), \quad \omega_{ij} \equiv \frac{1}{2}(F_{ij} - F_{ji}), \tag{11}$$

wher ρ and ρ_0 are the current and reference density, respectively.

4. Microstructural models of metal surface layers

Microstructural approach allows to describe an appearance and development of plastic anisotropy of metal element caused by large plastic deformations. On the microscopic level, the metal element is considered as an aggregate of grains which have a uniform crystallographic structure. The first effect, which leads to the plastic anisotropy, is a considerable grain elongation during a plastic yield. The elongated grains create something like material fibres of higher ductility in the metal element. This effect is called a morphological texture of metals. The second reason, which causes the plastic anisotropy, is the crystalline structure of metal grains. Because the plastic yield of a single grain appears as a result of glides on certain slip systems of grain crystallographic lattice, a grain behaviour is plastically anisotropic. For this reason, during a plastic yield, the slip planes and slip directions rotate together with the crystallographic lattice. In crystal aggregates, one can observe an appearance of privileged lattice orientations called a crystallographic texture. For pure metals, the crystallographic texture has decisive influence on an appearance and development of their plastic anisotropy.

The first complete formulation of single crystal plasticity has been proposed by Hill and Rice [15]. The model is based on the Schmid law: *a crystal yields when* *a shear stress on a certain slip system reaches some critical value.* The Schmid law plays a role of three-parameter piece-linear yield condition (Fig. 6). The corresponding flow rule is associated with this condition.

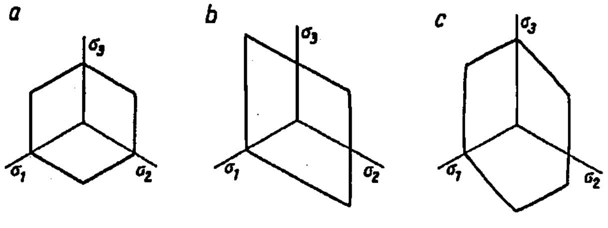

Fig. 6. Schmid yield surfaces for σ_3 directions: (a) $\langle 001 \rangle$, (b) $\langle 011 \rangle$, (c) $\langle 111 \rangle$.

A piecewise-linearity of the Schmid law leads to ambiguity in the choice of active slip systems at the plastic corners of yield surfaces. To avoid this problem, a viscous approximation of the plastic crystal behaviour is used in practice [16]. Recently, a real elastic-plastic model based on a regularization of the Schmid law has been proposed [17, 18]. Equations of the model have the following form:

$$\tau_{ij}^{\nabla} = \left(L_{ijkl} + \frac{f_{ij} f_{kl}}{f_{mn} g_{mn} + h_0} \right) d_{kl}, \tag{12}$$

where h_0 is a certain hardening parameter, and f_{ij}, g_{ij} are functions of the stress elastic moduli and lattice geometry of the crystal.

Models of single crystal behaviour enable to describe a behaviour of elastic-plastic polycrystals. It is possible owing to the Taylor assumption [19], which states that all local strain fields, in grains of a uniformly deformed polycrystalline specimen, are the same as a global macroscopic strain field. The above assumption allows to predict a texture evolution in a rolled metal surface layer (Fig. 7). The results presented in Fig. 7 have been obtained using the rigid-perfectly plastic model of the material. Equations (12) enable to formulate a finite element method (FEM) numerical code for prediction of texture evolution in deformed elastic-plastic metal elements [21].

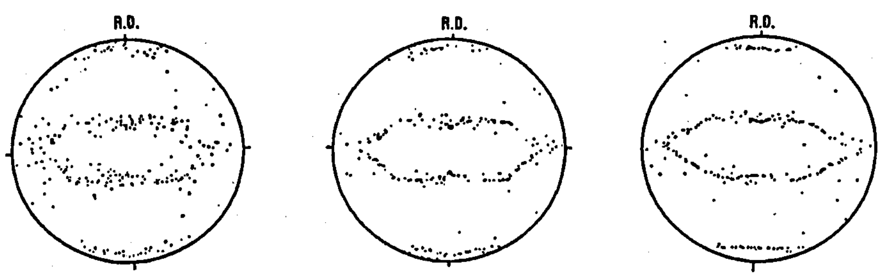

Fig. 7. The {111} pole figures for rolling of metal surface layer after 50%, 75% and 88% reduction of its initial thickness [20].

5. Conclusions

Mechanics of metal surface layers deals with problems which form three basic groups:

1 — experimental investigations, which are realized on

- the macroscopic level (measurements of material hardness and residual stresses in surface layers after non-mechanical treatments, and their changes after mechanical treatments);
- the microscopic level (description of geometrical and physical structure of the layers, mechanical tests of structure elements, description of structure changes after mechanical treatments);
- the submicroscopic level (measurements of dislocation densities on grain boundaries, investigation of formation and development of dislocation nets in plastically deformed surface layers);

2 — theoretical modelling, which includes

- a formulation and analysis of constitutive equations both on macro- and microscopic level;
- a formulation of initial-boundary problems describing a mechanical behaviour of surface layers;
- a formulation, development and application of numerical procedures for a simulation of surface layer behaviour during exploitation processes and mechanical treatments;

3 — identification procedures, which link together two above groups and look for

- a relation between a hardness and yield stress of surface layer;
- a relation between a hardness change and hardening of the layers;
- a relation between dislocation densities and latent hardening on slip systems of grains composing metal surface layers.

The last group of problems, which includes identification procedures, is the basic one for an engineering practice and still it is the least of all explored.

Acknowledgment

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