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YIELD STRESS DISTRIBUTION IN THE NATURAL SURFACE LAYER OF POLYCRYSTALS

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A metal surface layer of 2-3 grain diameters thick, before any technological treatment, without residual stresses and with a morphological structure the same as in the bulk material, is called *the natural surface layer*. Numerous tension tests with metal specimens demonstrate an earlier plastic yield of this layer [1–7]. The phenomenon may have an influence on the hardening and residual stress formation in metal surface layers during technological treatments of tools and machine elements. In the paper, a simple model of a yield stress distribution in the natural surface layer is proposed. The model is based on the fact that dislocation barriers on the free surface of grains are weaker than those on the grain boundaries in the bulk material. According to the model, the yield point in the layer may be 30% lower than in the bulk material. It enables us to explain the influence of the natural surface layer on the Young modulus measurements for thin metal specimens. The numerical calculations based on the proposed model are in agreement with the experimental observations [10–11].

1. Introduction

Properties of machine elements may be improved by formation on their surface of a thin layer of desirable features, which are different from those of the bulk material. Due to various metal surface technologies, one can obtain technological surface layers of thickness from over a dozen to several dozen grain diameters, which are more resistant to corrosion, wear and fatigue. These layers are more hardened than the bulk material and usually they are compressed by high residual stresses. To predict mechanical properties of the technological surface layers, it is necessary to know them in the primary state before any technological treatment.

Consider a macroscopically uniform and isotropic metal element without residual stresses. It is commonly observed [1–7], that a yield point of a surface layer of the metal element is lower than the yield point of the bulk material. This layer of 2-3 grain diameters thick will be called *the natural surface layer*. It is necessary to distinguish the natural surface layer of a polycrystalline material from the physical surface layer of single crystals

[8–9]. The last one appears due to oxidation of the free surface of single crystals, and its thickness is equal to few microns. In our considerations an influence of this layer on mechanical properties of the natural surface layer will be neglected.

In 1940, Glocker and Hasenmeier [1] have made X-ray tests of 0.01 mm thick surface layer of carbon steel. They have shown a reduction of the yield point in this layer up to 30 %. Independently, DAVIDENKOV [2] has analysed changes of the crystallographic lattice constant caused by an applied load. He has proposed the hypothesis about an earlier plastic yield of the near surface grains. The hypothesis has been confirmed by MACHERAUCH [3], who has compared the stresses in a specimen surface layer measured by means of the X-ray technique and the average stresses in the specimen measured in the classical tension test. Far below the yield point of the specimen, no differences were observed, but they appeared for higher loads. FUJITA and MIYAZAKI [4] have shown a dependence of the yield point on the number of grains in the specimen cross-section. From 2 to 48 grains have been considered. The results for the iron specimens of 0.025 mm in grain size are shown in Fig. 1.

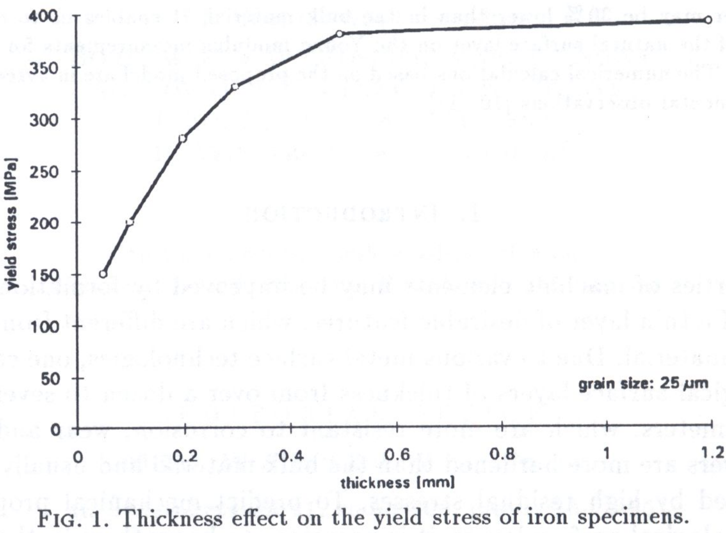

FIG. 1. Thickness effect on the yield stress of iron specimens.

GLIKMAN and others [1] have tested the appearance of residual stresses in tensioned specimens of carbon steel annealed at 870° C and tempered at 600° C. They noticed that the residual stresses were concentrated in a surface layer of thickness up to 0.2 mm. Their values as a function of applied displacements are shown in Fig. 2. The authors observed that, due to an earlier plastic yield of the surface layer, the layer was much more hardened than the remaining material. The last effect has been confirmed in other

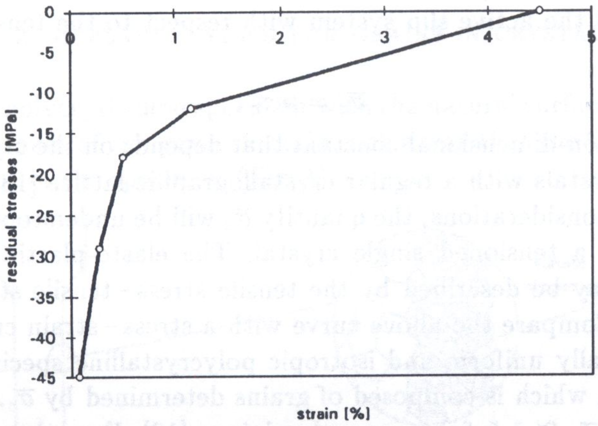

FIG. 2. Residual stresses in surface layer as a function of applied displacements.

papers [6 – 7].

The above phenomena take place in the natural surface layer of the tested specimens. The behaviour of a grain belonging to the layer seems to be intermediate between the single crystal behaviour and the behaviour of a grain taken from the bulk material of the specimen. In the next section, the mean yield stress of a tensioned single crystal and the yield stress of a polycrystalline specimen are compared. Next, plastic yield mechanisms in the grains of the natural surface layer lying at different depths are considered. The considerations lead to a model of the plastic behaviour of the grains. The model enables us to calculate the initial yield points for the successive grains of the layer. Two applications of the obtained rule are presented: yield stress distribution in the natural surface layer of aluminium specimen, and calculation of reduction of the Young modulus for thin metal specimens [10 – 11].

2. INITIAL YIELD POINT FOR SINGLE GRAIN AND POLYCRYSTAL

Consider the plastic yield of a single grain in tension. Let us assume that it appears due to a glide on one slip system. The slopes of the slip plane and the inclination of the slip direction to the direction of tension are denoted by angles χ and λ, respectively. The critical shear stress τ_c on the active slip system is connected with the tensile yield stress σ_c by the rule [12]:

$$\tau_c = \sigma_c \sin\chi \cos\lambda . \tag{1}$$

The quantity τ_c is a material constant, but σ_c depends on the angles χ and λ. Introduce $\overline{\sigma}_c$ as the mean value of $\sigma_c(\chi, \lambda)$ over all the possible orientations of the active slip system with respect to the tension direction. One can write

(2) $$\overline{\sigma}_c = m\tau_c,$$

where m is a non-dimensional constant that depends on the crystallographic lattice. For crystals with a regular crystallographic lattice [13], $m = 2.238$.

In further considerations, the quantity $\overline{\sigma}_c$ will be understood as the mean yield point of a tensioned single crystal. The elasto-plastic behaviour of this crystal may be described by the tensile stress – tensile strain averaged curve $\sigma - \varepsilon$. Compare the above curve with a stress – strain curve $\sigma - \varepsilon$ for a macroscopically uniform and isotropic polycrystalline specimen with the yield point σ_p, which is composed of grains determined by $\overline{\sigma}_c$. Experiments show that $\sigma_p/\overline{\sigma}_c \cong 1.5$ for a pure aluminium [12]. For other metals (iron, zinc) this ratio is much higher. Denote the difference between σ_p and $\overline{\sigma}_c$ by $2\sigma_b$ (Fig. 3). This difference is caused by an influence of grain boundaries on the plastic yield process.

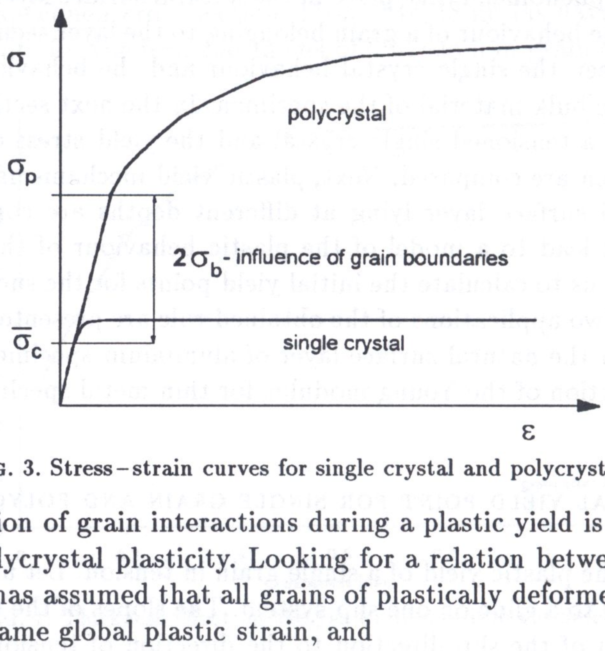

FIG. 3. Stress – strain curves for single crystal and polycrystal.

A description of grain interactions during a plastic yield is a basic problem of the polycrystal plasticity. Looking for a relation between σ_p and τ_c, TAYLOR [14] has assumed that all grains of plastically deformed polycrystal undergo the same global plastic strain, and

(3) $$\sigma_p = M\tau_c.$$

For f.c.c. metals, he has obtained $M = 3.06$. In the case of pure aluminium

(4) $$\sigma_p/\overline{\sigma}_c = M/m \cong 1.5,$$

in accord with the experimental results. Because for other metals the ratio $\sigma_p/\overline{\sigma}_c$ considerably exceeds the value 1.5, the quantities σ_p and $\overline{\sigma}_c$ will be considered in the further considerations as independent ones.

3. Mechanism of plastic yield for grains in crystal aggregate

Consider a polycrystalline specimen with the natural surface layer. Divide this layer into zones of one grain thick, in such a way that the first zone forms the free surface of the specimen (Fig. 4).

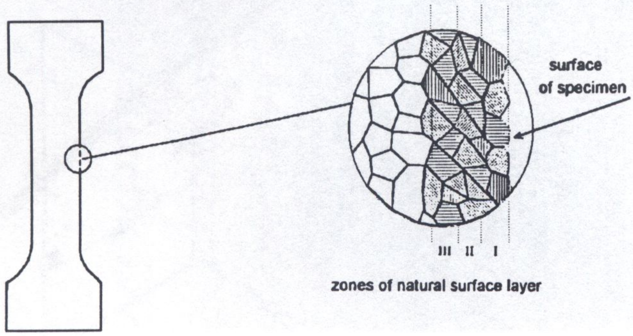

FIG. 4. Natural surface layer of polycrystal.

What is a behaviour of the successive zones during a tension process of the specimen? Due to lack of significant dislocation barriers on the specimen surface, the number of moving dislocations in the grains of the first zone will be considerably higher than that in the remaining zones. For that reason this zone undergoes the plastic yield first of all. On the other hand, the plastic yield of the first zone weakens the dislocation barriers on the border with the second zone. As a consequence, earlier plastic yield of the successive zones of the natural surface layer takes place.

Let us consider the mechanisms of plastic yield for: a single crystal, a grain situated far from the free surface of the specimen, and finally, a grain situated directly on the free surface of the specimen.

To plastify a single grain, the applied load should initiate a motion of a sufficiently large number of dislocations. To do it, the applied load should be large enough to overcome the dislocation barriers. The most important barriers are the following:

— stress fields caused by single dislocations and point defects, and in particular:

- dislocations and dislocation loops parallel to the slip plane,
- dislocations cutting the slip plane, i.e. a dislocation forest;

— stress fields caused by dislocation kinks.

The mechanism of plastic yielding for a grain situated in a polycrystal is more complicated. Grain borders create additionally very strong dislocation barriers (Fig. 5). A stress that produces a slip in a single grain is too small to do it in the grain situated far from the free surface of a polycrystalline

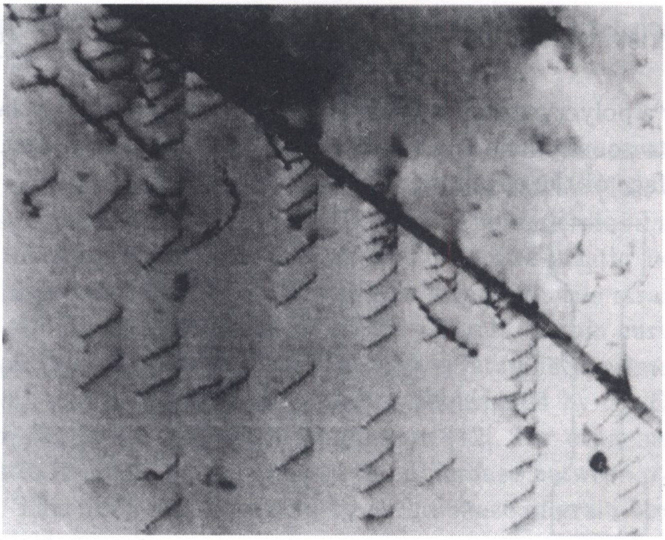

FIG. 5. Dislocation pile-ups on grain border. TEM microstructures of the samples after strain of 0.0113 (OLIFERUK, ŚWIĄTNICKI & GRABSKI [15]).

specimen. A dislocation behaviour in such a grain is shown in Fig. 6. Due to the load applied, dislocations propagate up to the grain border where they are blocked. In this way, the dislocation pile-ups are created, which are called superdislocations. For an increasing load, similar processes occur in other grains. Finally, the shear stresses at slip planes near the grain borders will be large enough to initiate slips in the neighbouring grains. During this process, new dislocations may appear due to nucleation on the grain borders or due to unlocking of the previously blocked dislocations.

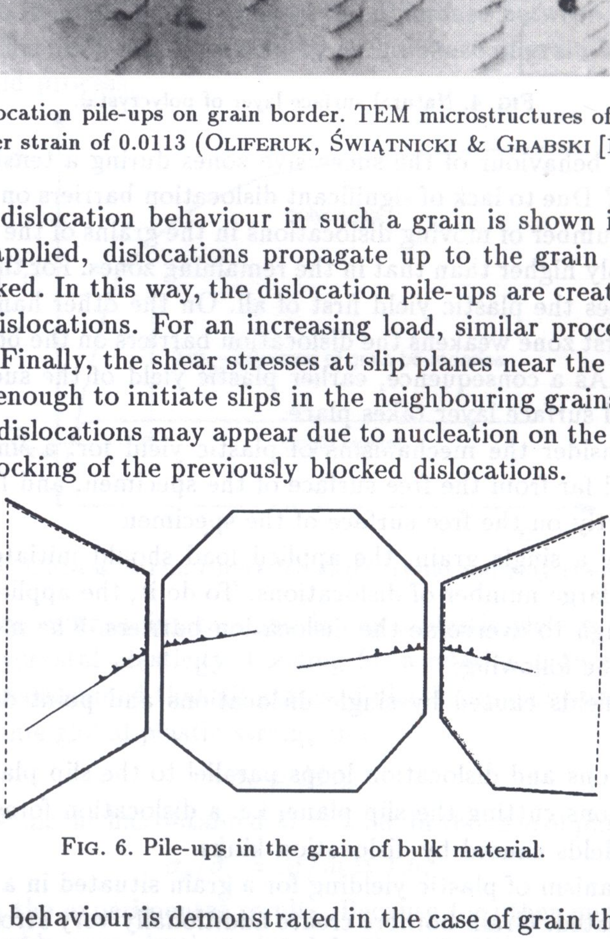

FIG. 6. Pile-ups in the grain of bulk material.

A different behaviour is demonstrated in the case of grain that belongs to the first zone of the natural surface layer. One side of this grain borders the free surface, and the second one – a grain of the next zone (Fig. 7). A dislocation motion in the considered grain is different because of its contact with the free surface. On the free side, dislocations may go out without making pile-ups. The situation is similar to that which occurrs in the case of the single crystal. However, on the opposite side of the considered grain, the dislocation motion is similar to that for the crystal situated deeply in the polycrystal.

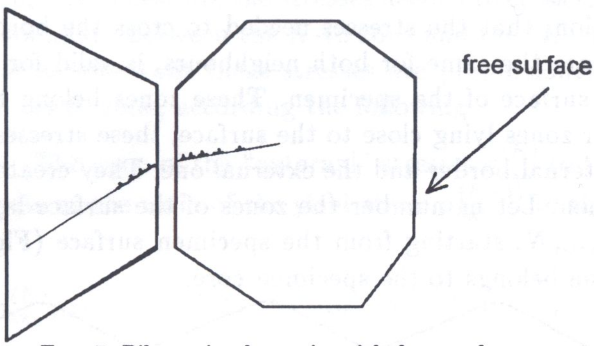

FIG. 7. Pile-up in the grain with free surface.

Concluding, the model of the natural surface layer will be constructed of three elements: *a single grain* in which the external surface does not create essential barriers for moving dislocations, *a grain from the polycrystal interior* that borders other grains considerably restricting the dislocation motion, and *a grain with a free surface* that is free on one side and adheres to the material on the other side. It will be assumed that the above elements represent grains with arbitrary lattice orientation, in plane strain state. For two first elements the averaged yield stresses are prescribed by $\overline{\sigma}_c$ and σ_p, respectively. The natural surface layer will be divided into several zones one grain thick. Modelling a successive zone, we will take into account the fact that a force that is necessary to overcome the dislocation barriers in this zone is proportional to the number of pile-ups, and then, to the yield stress in the neighbouring zone.

4. Model of natural surface layer

Consider a polycrystalline specimen with the natural surface layer. As previously, denote by $2\sigma_b$ the difference between the yield stress of the specimen σ_p and the averaged yield stress of the corresponding single crystal $\overline{\sigma}_c$. Let us take into account all crystals located at the same distance from the free surface of the specimen. They create a zone one grain thick (see Fig. 4). During a tension process, many superdislocations are concentrated on each of two borders of the considered zone. The average yield stress for this zone is

σ_p. It may be decomposed into two parts: $\overline{\sigma}_c$ and $2\sigma_b$. The quantity $\overline{\sigma}_c$ is the average yield stress of the zone without neighbours, while σ_b is an average stress that is necessary to overcome by superdislocations the borders of the zone. Then

$$\sigma_p = \overline{\sigma}_c + 2\sigma_b\,. \tag{5}$$

The assumption, that the stresses needed to cross the borders of the considered zone are the same for both neighbours, is valid for the zones lying far from the surface of the specimen. These zones belong to a core of the specimen. For zones lying close to the surface, these stresses may be different for the internal border and the external one. They create a surface layer of the specimen. Let us number the zones of the surface layer successively by $K = 1, 2, ..., N$, starting from the specimen surface (Fig. 8). Then, the $(N+1)$-th zone belongs to the specimen core.

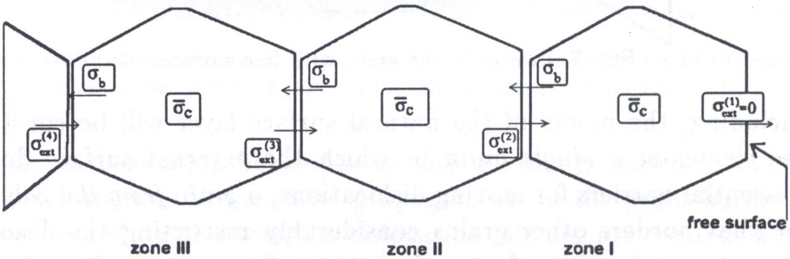

FIG. 8. Model of natural surface layer (arrows show directions of pile-ups' motion caused by corresponding stresses).

It seems to be quite natural to assume for all zones of the surface layer that the stresses needed to cross their internal borders by superdislocations are the same and equal σ_b. The assumption that these stresses are different for different zones gives differences smaller than 1%. On the other hand, the stresses needed to overcome their external borders will be, coming from the specimen core, smaller and smaller, and right on the specimen surface they will be equal to zero. Denote them by $\sigma_{\text{ext}}^{(K)}$, for $K = 1, 2, ...N$, keeping in mind that $\sigma_{\text{ext}}^{(1)} = 0$ and $\sigma_{\text{ext}}^{(N+1)} = \sigma_b$. Then, the total stress needed to plastify the K-th zone may be decomposed in the following way:

$$\sigma^{(K)} = \overline{\sigma}_c + \sigma_b + \sigma_{\text{ext}}^{(K)}\,. \tag{6}$$

In particular, for the first zone

$$\sigma^{(1)} = \overline{\sigma}_c + \sigma_b\,, \tag{7}$$

and for the first zone behind the surface layer

$$\sigma^{(N+1)} = \overline{\sigma}_c + 2\sigma_b\,. \tag{8}$$

According to the relation (5), $\sigma^{(N+1)}$ is equal to the yield stress of the specimen σ_p, and it is the same for all the remaining zones of the specimen core. Then, the yield stresses expressed by two known quantities $\overline{\sigma}_c$ and σ_p are determined in the whole specimen except the zones with numbers $K = 2, 3, ..., N$. To determine these unknown stresses, it is necessary to find $\sigma_{\text{ext}}^{(K)}$, for $K = 2, 3, ...N$. These are the stresses needed to cross the dislocation barriers on the boundary between the K-th zone and the $(K-1)$-th one (see Fig. 8). One can assume that these stresses are proportional to the yield stress of the $(K-1)$-th zone, according the following

HYPOTHESIS. The ratio of the "external" stresses $\sigma_{\text{ext}}^{(K)}$ to the "internal" ones σ_b is the same as the ratio of the yield stress $\sigma_{\text{ext}}^{(K-1)}$ to the yield stress σ_p, i.e.

$$\sigma_{\text{ext}}^{(K)}/\sigma_b = \sigma^{(K-1)}/\sigma_p \qquad \text{for} \quad K = 2, 3, ..., N. \tag{9}$$

For consistency of further considerations, it will be assumed that

$$\sigma^{(0)} \equiv 0. \tag{10}$$

The rules (5) – (6) and (9) – (10) lead to the following iterative formula:

$$\sigma^{(K)} = \overline{\sigma}_c + \frac{1}{2}(\sigma_p - \overline{\sigma}_c)(1 + \sigma^{(K-1)}/\sigma_p) \tag{11}$$

for $K = 1, 2, ..., N$. This formula is valid also outside the natural surface layer, for K higher than N. Notice, that for $K = 1$ and $K = N + 1$, Eqs. (7) and (8) are satisfied.

Concluding, we have found a yield stress distribution in the natural surface layer as a function of the global yield stress of the specimen σ_p, and the averaged yield stress of a single crystal $\overline{\sigma}_c$. According to the formula (11), in the successive zones of the natural surface layer, the yield stresses take the values

$$\begin{aligned}
\sigma^{(1)} &= \frac{1}{2}(\sigma_p + \overline{\sigma}_c),\\
\sigma^{(2)} &= \frac{1}{4}(3\sigma_p - 2\overline{\sigma}_c - \overline{\sigma}_c^2/\sigma_p),\\
\sigma^{(3)} &= \frac{1}{8}(7\sigma_p + 3\overline{\sigma}_c - 3\overline{\sigma}_c^2/\sigma_p + \overline{\sigma}_c^3/\sigma_p^2),\\
\sigma^{(4)} &= \frac{1}{16}(15\sigma_p + 4\overline{\sigma}_c - 6\overline{\sigma}_c^2/\sigma_p + 4\overline{\sigma}_c^3/\sigma_p^2 - \overline{\sigma}_c^4/\sigma_p^3),\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots
\end{aligned} \tag{12}$$

5. Yield stress distribution in the natural surface layer of aluminium specimen

As an illustration, the above rules will be applied to a specimen made of pure aluminium. In this case $\sigma_p/\overline{\sigma}_c \cong 1.5$ (see the rule (4)). Then, according to the formula (12), the yield stresses in the successive zones of the natural surface layer of the specimen will be the following:

$$
\begin{aligned}
\sigma^{(1)} &= 0.866\sigma_p ,\\
\sigma^{(2)} &= 0.982\sigma_p ,\\
\sigma^{(3)} &= 0.998\sigma_p ,\\
\sigma^{(4)} &= 1.000\sigma_p .
\end{aligned}
\tag{13}
$$

Notice that in the case of pure aluminium, the thickness of the natural surface layer is equal to $N = 3$ grain diameters, if the accuracy of calculations is 0.1 %. When the difference between $\sigma^{(K-1)}$ and σ_p is equal to 13.4 % in the first zone, it is smaller than 2 % in the second, and it drops to 0.2 % in the third zone. The results, in the form a continuous piece-wise linear distribution of the yield stresses, are shown in Fig. 9.

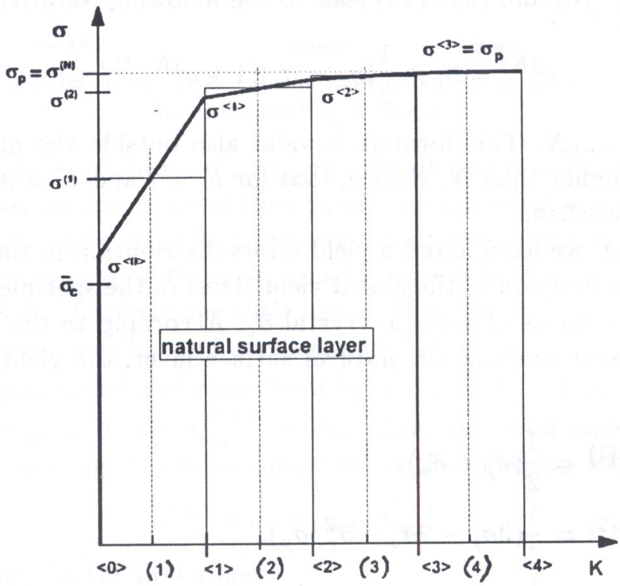

FIG. 9. Distribution of yield stresses in the natural surface layer of pure aluminium specimen.

They were obtained under the assumption that the calculated values $\sigma^{(K)}$ (index in round brackets) are valid in the zone centres. Denote by g

the thickness of the K-th zone, and by $\sigma^{<K-1>}$ and $\sigma^{<K>}$ (index in angle brackets) the yield stresses on the internal and external border of this zone, respectively. Then, the yield limit of the K-th zone is given by the rule:

$$\sigma^{(K)}g = \frac{1}{2}\left(\sigma^{<K>} + \sigma^{<K-1>}\right) g \tag{14}$$

that gives the following iterative formula:

$$\sigma^{<K-1>} = 2\sigma^{(K)} - \sigma^{<K>}. \tag{15}$$

For the last zone of the surface layer, the equalities hold true

$$\sigma^{<N>} = \sigma_p \qquad \text{and} \qquad \sigma^{<N-1>} = 2\sigma^{(N)} - \sigma_p . \tag{16}$$

For $K = N-2, N-3, \dots 1$, one can use the formula (15). The value of the yield stress on the specimen surface

$$\sigma^{<0>} = 2\sigma^{(1)} - \sigma^{<1>} \tag{17}$$

is always higher than $\overline{\sigma}_c$ (see Fig. 9). For the considered case, the yield stresses on the zone borders are as follows

$$\begin{aligned} \sigma^{<1>} &= 0.764\sigma_p, & \sigma^{<2>} &= 0.968\sigma_p, \\ \sigma^{<3>} &= 0.996\sigma_p, & \sigma^{<4>} &= 1.000\sigma_p. \end{aligned} \tag{18}$$

One can observe the reduction of the yield stress by 24 % on the specimen surface. In the case of carbon steel [1], the X-ray measurements of the surface layer of 0.01 mm thick have shown the drop of the yield stress up to 30 %.

6. Young's modulus dependence on specimen size

The proposed model of the natural surface layer enables us to explain why thin specimens made of the same material as the standard ones exhibit smaller values of Young's modulus than those obtained in the standard tests. To investigate this phenomenon, a dependence of the Young modulus on the surface-to-volume ratio F/V for cylindrical brass specimens of different radii r have been tested in [10 – 11]. The ratio $F/V = 2/r$ varied from 0.33 to 2.5. The Young moduli for the given and the standard specimens have been denoted by E and E_0, respectively. For a given F/V, the ratios E/E_0 were measured. The results are shown in Fig. 10. One can observe a distinct reduction of the Young moduli when the ratio F/V increases.

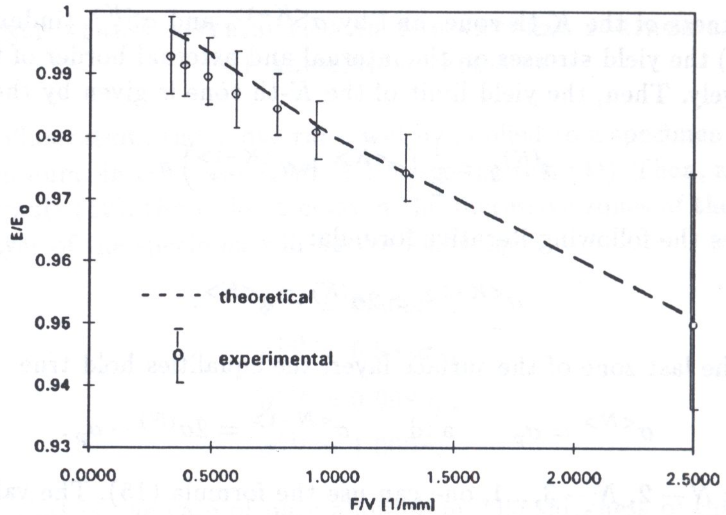

FIG. 10. Young's modulus dependence on the surface area-to-volume ratio for thin specimens.

The experimental results presented in [10] may be predicted with the help of the proposed model of natural surface layer. Consider a specimen with a large ratio F/V. Large ratio F/V denotes a small number of grains on the specimen cross-section and the large ratio of natural surface layer thickness to the thickness of the core. Then, the influence of the natural surface layer on the loading process compared with the influence of the core is considerable. During tension, when the core of the specimen is in an elastic range yet, the surface layer is in a plastic one. The load needed to obtain a prescribed specimen elongation is lower than that in the case of fully elastic specimen. As a consequence, the measured Young modulus is considerably lower than that in the case of a specimen with a thin surface layer. If the ratio F/V decreases, the number of grains in the cross-section increases and the influence of the natural surface layer on the specimen behaviour is negligibly small.

To investigate the influence of the natural surface layer on the Young modulus measurement, a simulation of the tension process has been done. To do it, a numerical code for elastic-plastic analysis of multilayered cylinder was used. The cylinder layers had different yield points. A detailed description of the model and algorithms of calculations were given in [16]. Considering the layers of tensioned cylinder as successive zones of natural surface layer, the yield stress distribution in the specimen was found. According to the paper [11], the calculations were performed under the assumption that the grain diameters were equal to 0.07 mm. It was assumed that $\sigma_p/\overline{\sigma}_c = 2.0$. Next, a tension test of the specimen in which its core remained elastic, was simulated. Specimens of different diameters but the same surface layer thicknesses were analysed. The results of calculations for specimens with the parameter $F/V = 2/r$ varying from 0.33 to 2.5 are shown in Fig. 10. They are very close to those obtained experimentally [10].

7. Conclusions

To describe rationally mechanical properties of metallic technological surface layers, a notion of the natural surface layer is essential. This is a layer that exists in a macroscopically isotropic and homogeneous metal element before application of any technological treatment. A characteristic feature that distinguishes the natural surface layer from the rest of material is its lower yield stress. This fact may have an influence on hardening and residual stress formation in metal surface layers during technological treatments of tools and machine elements. Moreover, taking into account the existence of the natural surface layer, one can explain such effects as a reduction of the Young modulus for thin specimens. A phenomenon of earlier plastic yield of the natural surface layer is caused by weaker dislocation barriers on the free surface of the material, and it was confirmed by many experimental tests [1-7].

In the paper, a simple model of the natural surface layer for polycrystalline materials was given. The surface layer was divided into zones of one grain thick. Taking into account the fact, that a force needed to overcome the dislocation barriers on the borders of the neighbouring zones is proportional to the number of piled dislocations, the initial yield stresses in the successive zones were found. According to the model, thickness of the natural surface layer is equal to 2-3 grain diameters. In the case of pure aluminium, the yield stress in the surface layer may be lower by up to 24 % of the yield stress of a whole specimen. The above results agree with the previous results of experimental tests [1-2]. As an application of the proposed model, the decrease of the Young modulus for thin cylindrical specimens is analysed. A numerical simulation of tension tests gives the result that is very close to the one obtained from the experiment for brass specimens [10-11].

Acknowledgments

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