Nanowires: diameter-dependent strength criterion

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Abstract. Kafka ś criterion of strength, published and substantiated in earlier author ś papers is applied to nanoscale wires with different thicknesses. The relation of the criterion parameters to the fineness of the material structure and to the quality of the surface is discussed.

1. Nomenclature

σ_{ij} = stress tensor
$\delta_{ij}\,\sigma$ = isotropic part of σ_{ij} ($\sigma = \sigma_{ii}/3$)
s_{ij} = deviatoric part of σ_{ij} $\left(s_{ij} = \sigma_{ij} - \delta_{ij}\sigma\right)$
ε_{ij} = strain tensor
$\delta_{ij}\,\varepsilon$ = isotropic part of ε_{ij} ($\varepsilon = \varepsilon_{ii}/3$)
e_{ij} = deviatoric part of ε_{ij} ($e_{ij} = \varepsilon_{ij} - \delta_{ij}\varepsilon$)
δ_{ij} = Kronecker's delta
ν = Poisson's ratio
$\mu = (1+\nu)/E$ deviatoric elastic compliance
$\rho = (1-2\nu)/E$ isotropic elastic compliance
E = Young's modulus
C = proportional strength limit
$D = CE$ (product of C and E, preferably used without necessity of determining C and E separately)
d = diameter of the wire
$r = d/2$

2. Introduction

Various strength criteria for yield or ultimate strength, such as Mohr-Coulomb criterion, Drucker-Prager criterion [1,2], Barton-Bandis shear strength criterion [3], Tresca criterion [4], Mises criterion [5], Matsuoka-Nakai failure criterion [6], Kafka strength criterion [7-13], etc. have been developed for general solid or special (laminated materials, rocks, etc.) materials. As for the nanoscale, Rubenstein [14] and Krasilnikov [15] have demonstrated that proportional strength of the nanofibers decreases

with the increase of their diameter. In the present study, Kafka´s strength criterion is shown to be applicable even on the nanoscale - to the description of this phenomenon.

3. Strength criterion

Kafka´s strength criterion results formally from a generalization of Mises´ yield criterion. The effect of the deviatoric part of the stress tensor is described as local and has the form of Mises´ criterion. The effect of the isotropic part of the stress tensor is described as non-local, resulting from the elastic energy comprised in a specific neighborhood (denoted Ω) of the most stressed parts of the surface (denoted L). Neighborhood Ω is specified as the area reaching up to a specific distance ω from the points of L. If the set of points with maximum exposure is limited to only one point in a 3D body, such neighborhood is spherical. If it is limited to only one point in a thin 2D plate, the neighborhood is circular. If this set forms a surface, an incasing layer of constant thickness forms the neighborhood.

Under these hypotheses, the criterion takes on the following form:

$$(w_d)_L + \kappa \{w_i\}_\Omega \le C, \tag{1}$$

where w_d means the elastic energy density of the deviatoric part of the stress tensor:

$$w_d = \tfrac{1}{2}\mu s_{ij} s_{ij}, \tag{2}$$

$(w_d)_L$ means the local value of w_d at the surface point (or points) of maximum exposure - locus L;

w_i means the elastic energy density of the isotropic part of the stress tensor:

$$w_i = \tfrac{3}{2}\rho\sigma^2, \tag{3}$$

$\{w_i\}_\Omega$ means the average value of w_i in neighborhood Ω specified above.

Usually (not always) the L-set of points with maximum exposure is on the surface, where the term $\left[(w_d)_L + \kappa\{w_i\}_\Omega\right]$ reaches its maximum value. Thus, the specific neighborhood Ω comprises some part of the loaded body and some part of free space.

For a constant value of E, it is advantageous to work with our criterion (1) in the following form:

$$\tfrac{1}{2}(1+\nu)\left(s_{ij}s_{ij}\right)_L + \kappa\tfrac{3}{2}(1-2\nu)\left\{\sigma^2\right\}_\Omega \le D \ (=EC), \tag{4}$$

where only the value of D is to be determined, without determining E and C separately.

The material parameters κ, ω and D depend on properties of the material of the investigated body and of its surface. The values of ω and D are positive. For κ the following relations hold true:

$\sigma > 0 \Rightarrow \kappa > 0, \quad \sigma < 0 \Rightarrow \kappa < 0, \quad \sigma = 0 \Rightarrow \kappa = 0$. If a part of the Ω-neighborhood is a free space outside the loaded body, the form of the Ω-neighborhood is not changed, but the value of w_i is vanishing in the free space, thus lowering the average value $\{w_i\}_\Omega$.

On the macro- and meso-scale, the usefulness of this criterion has been demonstrated in our previous papers [7-13], regarding the following problems:

- Pure shear strength of rivets ($w_i = 0$).
- Tension of wires with circular cross-sections and varying diameters – steel ($\kappa > 0$)
- Compression of prismatic specimens with varying size of their cross-sections – inorganic glass ($\kappa < 0$).
- Bending of plates with varying thickness – inorganic glass.
- Uniaxial compression of square plates with circular holes of varying diameters of the holes – inorganic glass and organic glass.

- Uniaxial tension of strips with circular holes with constant wideness of the strip and varying diameters of the holes – steel.
- Three-point bending of bars and tubes with circular cross-sections and varying size of the cross-sections.
- Size effect in the Brazilian split-cylinder test – concrete and inorganic glass

In all these cases, comparison of the outcome of Criterion (1) with experimental data gave good results and following findings:

(i) The higher the strength of the material and of the surface, the higher is the value of C

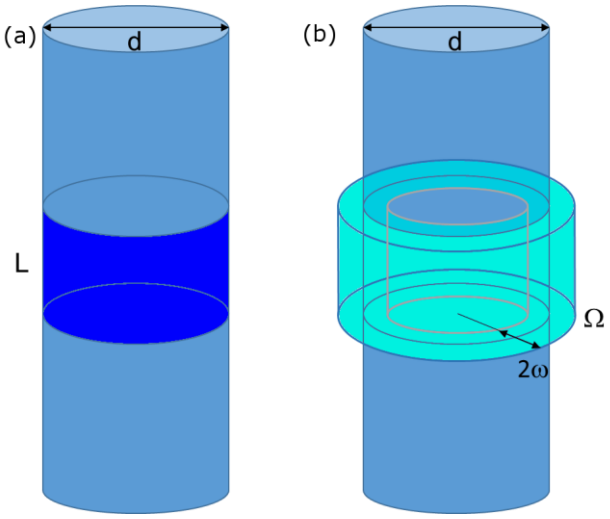
(ii) The higher the volume fraction and continuity of that material constituent that resists inelastic deformation, the higher is the value of ω

(iii) The higher the resistivity of the surface towards initiation of cracking (polished x unpolished surface), the higher is the absolute value of κ .

Application to nanowires

In this communication, applicability of the criterion even on the nanoscale is demonstrated. As an example, the experimental data presented in Rubenstein's paper [14] are used. In this paper, the strength of polycrystalline nickel wires has been investigated and the dependence of their proportional limit stress on their diameter demonstrated. This is similar to the problem of macroscopic wires in tension (Kafka, [8]). In Rubenstein ś paper [14], the experimentally found dependence is simulated by a curve-fitting formula. In our approach, the experimentally found dependence is shown to be describable by our physically substantiated criterion.

In the case of tension of common wires with circular cross-section, the set of points with maximum exposure L has the form of cylindrical surface of non-specified height, with radius $r = d/2$, (Figure 1a) and Ω has the form of a cylindical shell with thickness $2 \cdot \omega$ (Figure 1b), whose inner part with thickness ω covers a cylindrical part of the wire and the outer part (again with thickness ω) covers a part of free space. The value of w_i in this outer part is vanishing, thus lowering the average value $\{w_i\}_\Omega$.



(a) and neighborhood Ω (b) in the case of a wire with a diameter d.

Figure 1 The schematics of locus L

In Figure 1, the wire and objects L and Ω have a common longitudinal axis. For all the points of L, their distance from the axis is

$$r_c = d/2. \tag{A}$$

The value of w_i is here constant throughout the body, including locus L - the surface. The same is valid for w_d. The value of the left-hand side in Eq. (1) differs in different materials due to differing values of κ, ω. It differs also in wires of the same material, but with different thickness - due to fact that in this case the thickness *d* differs, but ω remains unchanged.

The Ω-neighborhood of the surface has tubular form – coaxial with the wire - whose thickness is 2ω. The radii of the inner and outer surfaces of Ω are:

$$r_i = d/2 - \omega \tag{B}$$

and

$$r_o = d/2 + \omega \tag{C}$$

In Eq.(1), the values of w_i and w_d between (A) and (C) are evidently vanishing, between (A) and (C) are given by Eqs.(2) and (3). The average value of $\{w_i\}_\Omega$ is then expressed as follows:

$$\{w_i\}_\Omega = \frac{\pi r_c^2 - \pi r_i^2}{\pi r_0^2 - \pi r_i^2} w_i = \frac{r_c^2 - r_i^2}{r_0^2 - r_i^2} w_i \tag{5}$$

Hence, our criterion takes into account not only the stress state, but also parameters κ and ω that depend on the material- and surface-quality. For different diameters of the wire, thickness 2ω of the Ω-neighborhood is the same; the value d of the diameter differs.

Using this concept, we can easily find such values of κ, ω and D that give the best description of the experimental points. The following values have been found for the experimental data presented by Rubistein [14]: $\kappa = 8000$ and $D = 2.8*10^5\ \mathrm{MPa}^2$ for both investigated structures of the material (fine and coarse, related to grain size of the tested material), ω=30 for the coarse structure and $\omega = 60$ for the fine structure. For these parameters, the course of our theoretical dependence of the proportional limit stress on the diameter of the wires is shown in Figure 2.

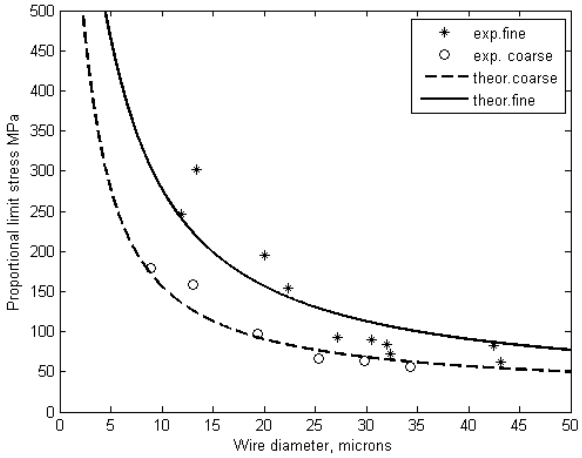


Figure2 Dependence of the proportional stress limit of the polycrystalline nickel wires on their diameter – experimental data according to Ref. [14].

Thus, the difference between the fine and the coarse structure is characterized by parameter ω (30 for the coarse structure and 60 for the fine structure). The fact that the values of the proportional limit stresses are higher for the fine structure than those of the coarse structure agrees e.g. with the findings presented by Krasilnikov [15], where the proportional limit stresses are found to be far higher than those presented by Rubenstein [14].

The reason why the value of ω is higher for the fine structure than that for the coarse structure can be explained as follows: The value of ω characterizes the extent of the area from which the stress state significantly influences the respective crack creation. This extent depends on the mechanical properties of the material:

- In a purely inelastic material, the extent is vanishing
- In a purely elastic material, the extent is theoretically unlimited, but the influence decreases with the distance from the crack locus; in our model this continuous decrease is simulated by a one-step decrease: from a constant to zero at the ω distance from the surface of the body.
- In a material with an elastic continuous grid, the extent depends on the properties of this grid, how dense, continuous and sturdy it is.

The dependence on the elastic grid is thoroughly discussed in Ref. [8]. In polycrystalline materials the resistant grid is represented by intergranular boundary areas, where irregularity of the crystalline structure prevents plastic deformation. It is evident, that in materials with fine structure, this grid is denser than in those with coarse structure, thus making the stress state nearer to the state in purely elastic material. This explains the higher value of ω in the material with fine structure.

In some materials (e.g. [16]) the experimentally detected Young ś modulus depends on the thickness of the wires. But even in such cases, our criterion is applicable; only the value of D is not constant, but depending on E; constant is here only C.

4. Conclusions

- Kafka's strength criterion is applicable even on the nanoscale.
- In a finer structure, the value of ω is higher due to the denser grid of a stronger material constituent - formed by the intergranular areas that are resistant to inelastic deformation.

Acknowledgements

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