The Influence of Random Microstructure Grain Size Distribution on the Deformation Properties of the Material

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Abstract. A mathematical model of micro-heterogeneous medium is created to investigate how the strength and deformational properties of a metal are affected by its grain size. The Hall-Petch relationship is applied with consideration to the randomness of grain diameters. Relative damage is determined through the probability of fracture in microstructure elements. Macro properties of the metal are calculated as they change due to micro fractures. Stress-strain curves are constructed while taking into account the changing microstructural damage at each increment of deformation. A comparison is made with experimental diagrams for copper with several average grain diameters. The purpose of this article is to create a mathematical model that takes into consideration the influence of the random grain size distribution on the deformational and strength properties of the metals.

INTRODUCTION

The statistical metallurgy studies effects of random microstructure properties on deformational and strength properties of metals [1-3]. The heterogeneity of metal properties at the micro level justifies the use of probability theory in calculations. One of the characteristic properties of metal is the connection between its deformational properties and the grain size of its microstructure. This interaction is expressed by the relationship of Hall-Petch [4,5]. At nano level, a reversed Hall-Petch effect may be observed that means as the average grain diameter decreases, the resistance of the metal to rupture and its yield strength also decrease. This particular study investigates the level of microstructure at which the effect of Hall-Petch is direct. Microstructure grain diameters deviate from their average size. The Hall-Petch relationship will be considered as a function of the random microstructure grain diameter.

Let a model of a micro-heterogeneous medium [1, 2] contain elements of two orders of infinitesimal. Elements at the macro level have deterministic mechanical properties. Microstructure elements are second order infinitesimal and have random deformational and strength properties. For microstructure elements at points $X = (x_1, x_2, x_3)$ the random Young modulus $E(X)$, and the deterministic Poisson ratio ν are considered. Calculation of macroscopic properties of a material as a function of the properties of its microstructure elements is one of the main goals of the micro-heterogeneous media theory . Tensor of adjustments h reflecting microstructure elements interaction is added to the tensor of average elastic moduli C [1,2]. The adjustment tensor h depends on the moment functions of random microstructural elastic moduli. As a result, the adjusted Young's macro modulus $\tilde{E}$ and the Poisson's ratio $\tilde{\nu}$ are calculated. For calculating of the elastic macro-moduli this article uses the calculation methods developed in the article [2].

RANDOM DISTRIBUTION OF GRAIN DIAMETERS

The Hall – Petch relationship [4,5] illustrates the connection between the yield strength of a polycrystalline material σ_y and its grain diameter d:

$$\sigma_y = \sigma_0 + \frac{k}{\sqrt{d}}, \tag{1}$$

where σ_0 is a stress required for a dislocation onset in a monocrystalline solid, and k is a constant specific to each material. The coefficient k quantifies the growth of the polycrystalline material yield strength with the decreasing grain size. Consequently, with increasing grain size the yield strength decreases. A similar relation to the grain size is also characteristic to the tensile strength of metals [7].

The randomness of grain sizes is one of the reasons for heterogeneity in the microstructure properties. Let $f(x)$ be defined as a probability distribution density for grain diameter x. Let variable y be the yield strength of microstructure grains. Then to find the distribution density $g(y)$, we use equations for probability distribution density of a function of a random variable.

Consider two monotonic mutually inverse functions with parameters a and b: $y = \varphi(x)$ and $x = \psi(y)$:

$$y = \varphi(x) = a + \frac{b}{\sqrt{x}}, \quad x = \psi(y) = \frac{b^2}{(y-a)^2}, \quad \psi'(y) = \frac{-2b^2}{(y-a)^3}, \tag{2}$$
$$g(y) = f(\psi(y))\,|\psi'(y)|.$$

If the grain diameter x has a normal distribution with expected value m and the standard deviation s, then the probability density distribution of the grain tensile strength $g(y)$ is

$$\mathrm{g}(y,m,s,a,b) = \frac{1}{s\sqrt{2\pi}} \cdot \frac{2b^2}{(y-a)^3} \exp\left(-\frac{\left(b^2 - m(y-a)^2\right)^2}{2s^2(y-a)^4}\right). \tag{3}$$

The distribution density of the microstructural strength conditions is used to calculate the microstructure damage.

THE RELATIONSHIP BETWEEN STRAIN AND STRESS

The difference between the stress $\sigma(X)$ and the random tensile strength $S(X)$ in a grain $X = (x1, x2, x3)$ is defined as: $w(X) = \sigma(X) - S(X)$. The random function $w(X)$ is a microstructural strength condition. $S(X)$ can also be a yield strength depending on the problem setup and requirements. If $w(X) \geq 0$, then the stress at the point X is greater than the strength; therefore, the element of the microstructure will sustain fracture. If $w(X) < 0$, the fracture does not occur since the stress is in the safe range. The methods for calculating the random microstructural stress $\sigma(X)$ are explored in the article [2]. Here only the deterministic value of the macro stress σ will be considered. In the process of loading, the stress σ increases and the microstructure damage accumulates. The condition for the grain fracture is $S(X) \leq \sigma$. Parameter q defines the damage or the relative number of fractured microstructure elements. Let $g(\sigma)$ be the probability distribution density of the microstructural strength calculated with the Hall – Petch relationship. The formula for assessing damage $q(\sigma)$ under variable stress σ takes the following form:

$$q(\sigma) = \int_{-\infty}^{\sigma} g(y)\,dy = \int_{-\infty}^{\sigma} f(\psi(y))\,|\psi'(y)|\,dy = \int_{0}^{\psi(\sigma)} f(t)\,dt. \tag{4}$$

Micro-fractures gradually change the elastic macro-modules. The relationship between deformations and stresses of the material also changes as a result.

In the process of loading, the onset and the subsequent accumulation of material damage is observed in a structure. The deformation properties of the metal gradually change. The material deformation diagrams are significantly affected by the properties of the microstructure [2] including the microstructure grain size. The type of probability distribution of random grain size affects the process of the microstructure damage. Considering the damage of the microstructure q at each stage of loading, the macro properties of the material are recalculated. New properties of the material reflect the equilibrium state to which the microstructure has returned after it sustained micro damage.

Let us calculate the uniaxial tension diagram while taking into account random properties of microstructure elements. In the process of loading, the incremental increases of the stress $\Delta\sigma$ are considered. At each (i + 1) step the macro deformation ε_{i+1} is determined by the expression that contains the macro module $\tilde{E}_i$, a macro-modulus calculated for the damage sustained in the previous step. Using small incremental increases $\Delta\sigma$, the integral relationship between the strains $\varepsilon(\sigma)$ and stresses σ is derived.

$$\varepsilon(\sigma) = \int_0^{\sigma} \tilde{E}(z)^{-1} dz. \tag{5}$$

The diagram is terminated when the critical levels of material loading are exceeded [2].

NUMERICAL EXAMPLE

Let us use a numerical example to find out the influence of the distribution parameters of a random microstructure grain size on the relationship between stresses and strains in a metal. Consider the experimental data by Bilello and Metzger listed in [8] (Bilello, Metzger, 1969) for tension in five samples of polycrystalline pure copper with different grain sizes. The experiments were structured in the context of microplasticity, and the nonlinear relationship between small deformations and stresses was studied. The average grain diameters d of the samples were 50 μm, 150 μm, and 380 μm. As the samples with a cross section area of 3 mm^2 were loaded in tension, the graphs of the nonlinear relationship between stresses σ (kgf / mm^2) and strains ε in the (σ , $\sqrt{\varepsilon}$) axes were derived for small strains up to ε = 0.002. The coordinates of the experimental graphs for the three average grain diameters d are converted from axes ($\sqrt{\varepsilon}\cdot 10^3$,σ (kgf/mm^2)) to the axes (ε, σ(MPa)) and gathered in the Table 1.

σ MPa		4	6	8	10	12	14	16	18
d = 50 μm	$\varepsilon\cdot 10^4$	0.04	0.2	0.6	1.4	2.9	6.5	10	20
d = 150 μm		0.01	0.04	0.2	0.6	1.4	3.1	6.8	11
d = 380 μm		0	0.01	0.06	0.3	0.7	2.1	4.6	9.9

Table 1. The relationship between stresses σ (MPa) and strains ε in polycrystalline copper for various average grain diameter d.

Let us calculate the parameters of the Hall-Petch relationship using experimental data. The average value of the grain strength S is assumed to be equal to the macroscopic yield strength. This condition usually corresponds to the stress reached at the strain ε = 0.002. Based on Table 1 for d = 380 μm obtain S = 18.2 MPa. Through extrapolation of the 2nd and the 3rd rows arrive at S = 20.5 MPa for d = 150 μm and S = 22.3 MPa for d = 50 μm. The Hall-Petch relationship linearly depends on $d^{-0.5}$ as $S = a + b\cdot d^{-0.5}$. Hall–Petch constants a and b are calculated using three points ($d^{-0.5}$, S) with the method of the ordinary least squares. Fig. 1 shows the resulting Hall – Petch relationship for points (0.14, 22.3), (0.082, 20.5), (0.051, 18.2). The resulting relationship is

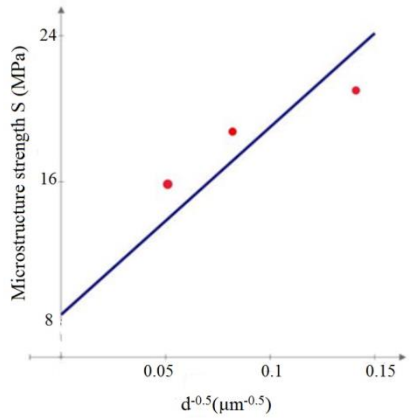
$$S(d) = 12.5 + \frac{82}{\sqrt{d}}. \tag{6}$$

The probability distribution density $f(x)$ of a random grain diameter x can be determined through examination of polished specimens of the material [1,3]. This problem has not been addressed in experiments [8]; therefore, let us consider some hypotheses about the random characteristics of grain diameters with expected values of 50 μm, 150 μm, and 380 μm. Let these be the normal distribution with the expected value m and the standard deviation s. Using the relationship (6), the corresponding densities (3) of the distribution $g(y)$ of the microstructure grain strength are found. With an increase in the expected value of the random strength S, the probability of micro fractures decreases. The relative damage, that is also the probability of microstructural fractures, is calculated with the formula (4). Also, worth noting that with a smaller variance of the random variable the damage accumulates more slowly, and the material withstands higher stresses [2].

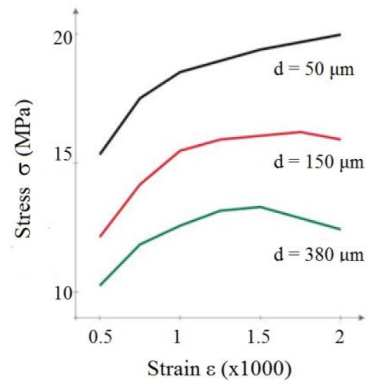
Let us proceed to the calculation of the relationship between deformation and stress when the Hall-Petch relationship for a given material and the distribution parameters of the random grain size are known. Using data from Table 1 for an intact material, let the Young's modulus E = 122 GPa. The Poisson's ratio for copper is ν = 0.34.

Having determined the material damage $q(\sigma)$, the adjusted Young's modulus $\tilde{E}$ is recalculated using the functions (3,4) with parameters $E, \nu, a, b, s,$ and m. These parameters, as well as the type of distribution of the grain size, affect the shape of the stress-strain curve of the material.

Let us consider three different average values m with the same coefficients of variation $\frac{s}{m} = 0.20$. Then for m = 50 μm, m = 150 μm, and m = 380 μm, it is obtained that s = 10 μm, s = 30 μm, and s = 72 μm respectively. Using formulas (5), the stress-strain diagram for each of the three cases is constructed. Fig. 2 represents the results of the calculations. The graphs show the distinctive influence of the microstructure grain size on the relationship between stresses and strains under loading.



(1)



(2)

FIGURE 1. The relationship between the average microstructure grain strength *S* and the value of $1/\sqrt{d}$ where *d* is the average grain diameter. The dots mark the experimental data.

FIGURE 2. Stress-strain curves for copper with different average grain diameters *d*.

CONCLUSION

A methodology for constructing a metal deformation diagram with consideration to the grain size of the microstructure has been developed. The Hall-Petch relationship is considered as a function of the random grain size and is used to calculate the random microstructural strength and the relative damage of the metal. A numerical example using experimental data on the deformation of copper with different average grain diameters is given. The results show that the shape of the stress-strain curve is influenced by the properties of the microstructure, including the probability distribution parameters of its grain size.

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