M2D2017

Proceedings of the
7th International Conference on
MECHANICS AND MATERIALS IN DESIGN

(Albufeira/Portugal, 11-15 June 2017)

Editors

J.F. Silva Gomes and Shaker A. Meguid

FEUP-INEGI

(2017)

Proceedings of the 7th International Conference on Mechanics and Materials in Design,
Albufeira/Portugal 11-15 June 2017. Editors J.F. Silva Gomes and S.A. Meguid.
Publ. INEGI/FEUP (2017)

PAPER REF: 6597

INFLUENCE OF GRAIN SIZE DISTRIBUTION ON THE MECHANICAL BEHAVIOR OF MATERIALS IN A WIDE RANGE OF STRAIN RATES

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ABSTRACT

This work compares the mechanical behavior of alloys with influence of grain size distribution on the in a wide range of strain rates. Constitutive model was proposed for describing the inelastic deformation and damage of alloys with face centered cubic and hexagonal close packed structures and distribution of grain sizes. It was shown that the dependences of the yield stress on logarithm of normalized strain rate for aluminium and magnesium alloys with a bimodal distribution of grains and coarse-grained alloys are similar. The yield stress at room temperature of the magnesium and aluminium alloy increased on 10 - 15 % in comparison with a coarse-grained alloy if the volume fracture of the UFG grains is close to the percolation threshold.

Keywords: grain size, high strain rates, light alloys, bimodal grain size distribution, strength, ductility, ultrafine-grained alloy, aluminium, magnesium.

INTRODUCTION

In recent years, the interest in the question of the impact of grain structure on the mechanical properties of metals and alloys increased continuously. Technologies of severe plastic deformation (SPD) allow creating an ultrafine-grained structure with a unimodal and bimodal distribution of grain size in metals and alloys.

By improving the Electron Backscattering Diffraction (EBSD) method was received new data on the texture formation and the evolution of a grain size distribution in coarse grained and ultrafine-grained metals and alloys under different impacts (Cayron, 2006, Sakai, 2014, Tiamiyu, 2016).

It was shown that nanostructured and ultrafine-grained metals and alloys have excellent physical and mechanical properties significantly superior the strength over their coarse-grained counterparts (Valiev, 1991, 1993, Herzig, 2008, Skripnyak, 2012, Garkushin, 2015, Li, 2017).

Steels and alloys with a bimodal grain size distribution demonstrate a unique combination of high yield and ultimate strength with satisfactory plasticity (Pozdnyakov, 2007, Malygin, 2008, Valiev, 2010, Dapeng, 2011). These materials are becoming increasingly important in the development of advanced construction techniques.

The influence of the grain size distributions on mechanical behavior of metal alloys at high strain rates and intense dynamic effects are not studied systematically. It was shown the influence of average grains size on the yield stress at compression and tension was established earlier for aluminium, titanium, and magnesium alloys.

It was found that with a decrease in the average grain size of metals and alloys to less than several microns, the flow stress at room temperature of metal alloys is increased, but the elongation to fracture is reduced (Prasad, 2009, Valiev, 2010, Dapeng, 2011). Light alloys with a bimodal grain size distribution possess a negative strain rate sensitivity of the yield stress and higher ductility at quasi static loadings (Fan, 2006, Ahn, 2008). Cracks growth resistance in UFG alloys with a bimodal grain size distribution increases due to deflection of microcracks on borders between UFG and coarse grained (CG) regions. Distribution effect of grain size on the mechanical behaviour of light alloys at high strain rates have been investigated insufficiently.

The aim of this study was to obtain estimates of the impact of the distribution of the grain size on the mechanical behavior of the alloys in a wide range of strain rates.

COMPUTATIONAL MODEL

Mechanical behavior of coarse grained and ultrafine-grained polycrystalline alloys can be described by the constitutive equations with explicit accounting for the effective grain size (Herzig, 2008, Skripnyak, 2012, Lim, 2011). Constitutive equations developing in the framework of continuum damage mechanics is convenient to use for solution of dynamic problems (Herzig, 2008, Skripnyak, 2012, Wang, 2013).

The constitutive equation can be used in the form

$$\sigma_{ij} = \sigma_{ij}{}^{(m)}\varphi(D),\ \sigma^{(m)}{}_{ij} = -p^{(m)}\,\delta_{ij} + S_{ij}{}^{(m)}, \tag{1}$$

where σ_{ij} is components of the Cauchy stress tensor, p is the pressure, S_{ij} is components of the deviatoric stress tensor, the superscript m indicates the condensed phase of the damaged material, φ (D) ≈1 - D is the function of damage, and D is the damage parameter.

The local damage parameter D is introduced to the material particle of a continuous medium or of a representative volume of the material:

$$D = \int_0^{t_f} \frac{\dot{\varepsilon}^n_{eq}}{\varepsilon^n_f}\, dt \tag{2}$$

where $\dot{\varepsilon}^n_{eq} = (\frac{2}{3}\dot{\varepsilon}^n_{ij}\dot{\varepsilon}^n_{ij})^{1/2}$, $\dot{\varepsilon}^n_{ij}$ is a components the inelastic strain rate tensor, ε^n_f is a strain to fracture, t_f is a loading time.

The bulk inelastic strain rate can be calculated by relation:

$$\dot{\varepsilon}^n_{kk} = \frac{1}{3}\frac{\dot{D}}{(1-D)}, \tag{3}$$

where symbol «·» denote the time derivative.

The pressure is calculated by equation of state (McQueen, 1960, Fomin, 2004). The deviatoric stress is calculated by the equation:

$$DS_{ij}^{(m)} / Dt = 2\mu(\dot{e}_{ij} - \dot{e}_{ij}{}^{n}), \tag{4}$$

where D/Dt is the Jaumann derivative, μ is the shear modulus, $\dot{e}_{ij}$ is the deviator of the strain rate tensor, and $\dot{e}_{ij}^{n}$ is the deviator of the inelastic strain rate tensor.

The deviator of the inelastic strain rate tensor is written as:

$$\dot{e}_{ij}^{n} = (3/2)[S_{ij}\,\dot{e}_{eq}^{n} / \sigma_{eq}], \tag{5}$$

where $\sigma_{eq} = [(3/2)S_{ij}^{(m)}S_{ij}^{(m)}]^{1/2}$ is the equivalent shear stress.

The plastic deformation of metals and alloys depends on the strain, the strain rate and the deformation temperature. Therefore the flow stress can be written as:

$$\sigma_s = \sigma_s\left(\varepsilon_{eq}^{n}, \dot{\varepsilon}_{eq}, T\right), \tag{5}$$

where ε is the true strain, $\dot{\varepsilon}_{eq} = [(2/3)\dot{\varepsilon}_{ij}\dot{\varepsilon}_{ij}]^{1/2}$ is the equivalent true strain rate, and T is temperature.

The yield stress can be predicted using the modified Zerilli -Armstrong constitutive model for alloys with Face Centered Cubic structure (FCC), Body-Centred Cubic structure (BCC), and Hexagonal Close Packed (HCP) structure (Zerilli, 1992):

$$\begin{aligned}\sigma_s = \sigma_{s0} + [C_6 d_g{}^{-1/2} + C_5(\varepsilon_{eq}^{p})^{n_1}]\exp[-T\ln(\dot{\varepsilon}_{eq}/\dot{\varepsilon}_a)] + \\ + C_1\exp[-C_3T + C_4T\ln(\dot{\varepsilon}_{eq}/\dot{\varepsilon}_b)]\end{aligned} \quad \text{(HCP alloys)}, \tag{6}$$

or

$$\begin{aligned}\sigma_s = \sigma_{s0} + C_6 d_g{}^{-1/2} + C_2(\varepsilon_{eq}^{p})^{1/2}\exp[-C_3(1 - \ln\dot{\varepsilon}/\ln\dot{\varepsilon}_b)T] + \\ + C_4[\varepsilon_r(1 - \exp(-\varepsilon_{eq}/\varepsilon_r))]^{1/2}\exp[-TC_7(1 - \ln(\dot{\varepsilon}_{eq}/\ln\dot{\varepsilon}_a))]\end{aligned} \quad \text{(HCP alloys)}, \tag{7}$$

$$\sigma_s = \sigma_{s0} + C_6 d_g{}^{-1/2} + C_5(\varepsilon_{eq}^{p})^{n_1} + C_1\exp[-C_3T + C_4T\ln(\dot{\varepsilon}_{eq}/\dot{\varepsilon}_{eq0})] \quad \text{(BCC alloys)}, \tag{8}$$

$$\sigma_s = \sigma_{s0} + C_6 d_g{}^{-1/2} + C_2(\varepsilon_{eq}^{p})^{1/2}\exp[-C_3T + C_4T\ln(\dot{\varepsilon}_{eq}/\dot{\varepsilon}_{eq0})] \quad \text{(FCC alloys)}, \tag{9}$$

where C_1, C_2, $C_3(d_g)$, $C_4(d_g)$, C_5, C_6, C_7, n_1, ε_r, $\dot{\varepsilon}_a$, $\dot{\varepsilon}_b$ are material constants, T is the temperature of loading in Kelvin, d_g is the average size of grains.

Estimation of effective grain size d_g in ultrafine-grained alloys or alloys with a bimodal distribution of grains sizes requires a detailed analysis of the grain structure of the alloys. Grain size distribution in steels and metal alloys can be determined by Electron Bakscattering Diffraction (EBSD) method. The EBSD map of the grain size after ECAP of 1560 aluminium alloy is shown in Fig. 1. Studies of the grain structures was carried out by EBSD method (DOE) using the electron microscope Tescan Vega II LMU (Moskvichev, 2016).

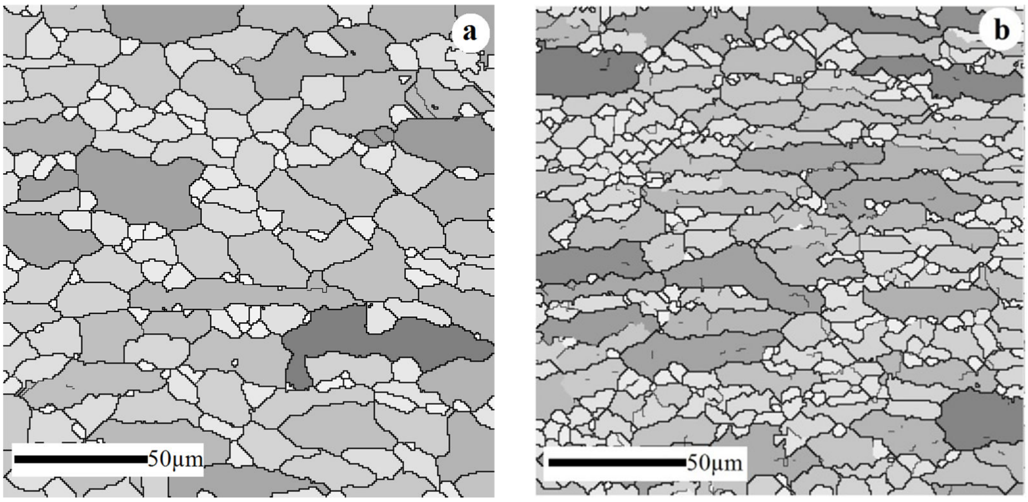

Fig. 1 - EBSD maps of the grain structure of aluminium alloy 1560 (a) as-received condition, (b) after 4 cycles of groove pressing technique

Analysis of the distribution of grain size of metallic alloys have shown that there are several characteristic types of distributions: unimodal, bimodal and multimodal distributions. Unimodal distribution of grain size in metals can be described by the formula log normal distribution (Berbenni, 2007):

$$f_k(d_g) = \frac{1}{\sqrt{2\pi}\, d_g S_n} \exp[-\frac{1}{2}(\frac{\ln(d_g / d_{gm})}{S_n})^2], \tag{10}$$

where d_g is the grain size, $d_{g\ m}$ is the median grain size of the distribution and S_n is the standard deviation in a number weighted grain size distribution.

The distribution of the grain sizes of aluminium alloy 1560 (a) for as-received condition, and (b) after after 4 cycles of groove pressing technique is shown in Fig. 2.

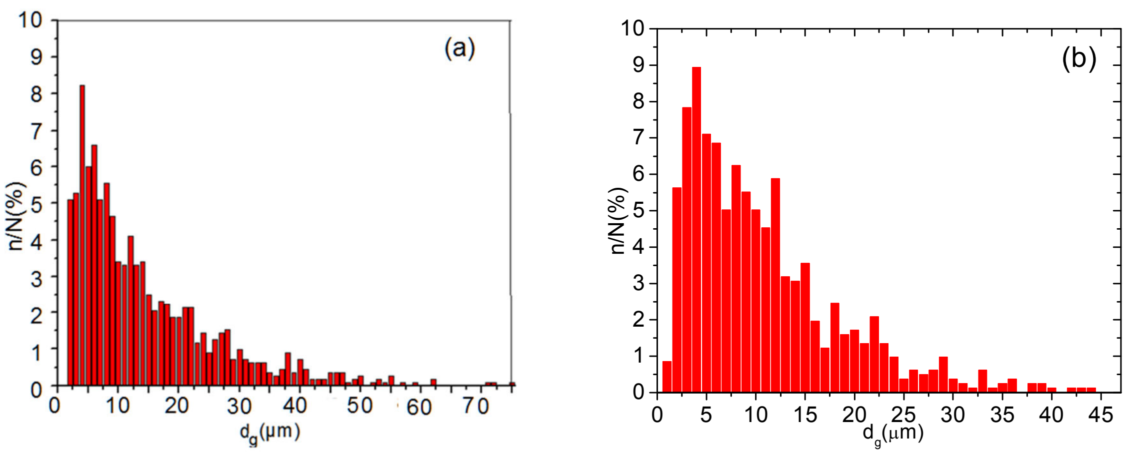

Fig. 2 - Distribution of the grain sizes of aluminium alloy 1560: (a) - as-received condition, (b) - after 4 cycles of groove pressing technique

The Weibull distribution function can be used for description of the unimodal distribution of grain size in metal alloys (Skripnyak, 2012, 2014, 2015):

$$f_k(d_g) = f_0 + \frac{b}{a}\left[\frac{d_g - c}{a}\right]^{b-1} \exp\left[-\left(\frac{d_g - c}{a}\right)^b\right], \tag{11}$$

where d_g is the grain size, b is the shape parameter, a is the scale parameter, and c is the location parameter of the Weibull distribution function.

The bimodal or multimodal probability density function can be presented as sum of probability density function of coarse grains, fine grains, and ultra fine grains:

$$f(d_g) = \sum_{k=1}^{m} \lambda_k f_k(d_g), \quad \sum_{k=1}^{m} \lambda_k = 1, \tag{12}$$

where d_g is the grain size, $f_k(d_g)$ is the unimodal probability density functions of grain size distribution, λ_k is weighting coefficients.

A multimodal distribution of the grain sizes of aluminium alloy 1560 after 4 cycles of groove pressing technique is shown in Fig.3

The specific volumes of UFG (with grain size 50 nm < d_g < 1 μm fine grains (1 μm <d_g<10 μm), and coarse grains (10 μm <d_g< $d_{g\ max}$) are described using probability density functions f_1, f_2, f_3 of UFG, FG, and CG grain systems, respectively:

$$C_{UFG} = \int_{d_g^{min}}^{1\mu m} f_1(x)dx, \quad C_{FG} = \int_{1\mu m}^{10\mu m} f_2(x)dx, \quad C_{CG} = \int_{10\mu m}^{d_g^{max}} f_3(x)dx, \tag{13}$$

where C_{UFG}, C_{FG}, C_{CG} are the volume fraction of ultra fine grains, fine grains and coarse grains, respectively.

Statistical samplings of large and fine grains can be combined into a single sampling. In this case, the distribution of grains sizes is considered as bimodal distribution.

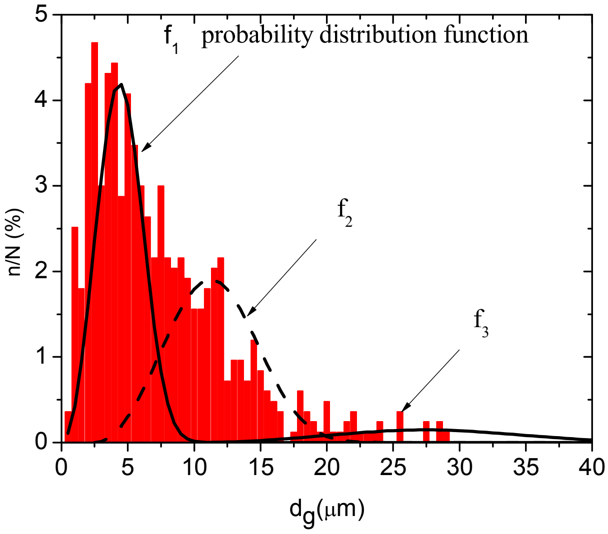

Fig. 3 - Multimodal distribution of the grain sizes of aluminium alloy 1560 after after 4 cycles of groove pressing technique

The volume fraction of coarse grains C_{CG} ≈0.363 corresponds to the percolation threshold of large grains in the representative volume of the material (Skripnyak, 2014, 2015).

Metal alloys with the volume fraction of coarse grains in the range 0.363 < C_{CG} <0.637 have some similarities with composite materials. The average grain size or the effective grain size are used for prediction grain-size hardening of polycrystalline alloys after the pioneering research of Hall and Petch (Valiev, 1993).

The average grain size can be defined for unimodal distributions of grain size and effective grain size is used for bimodal or multimodal distributions of grains sizes.

The average grain size $\overline{d}_g$ was related to the median grain size d_{gm} of unimodal grain size distribution (Zhu, 2005, Gollapudi, 2012):

$$\overline{d}_g = d_{gm} \exp(S_n^2 / 2), \tag{14}$$

where d_g is the grain size, d_{gm} is the median grain size of the distribution and S_n is the standard deviation in a number weighted grain size distribution (See Eq. (1)).

The effective grain size $d_{g\,eff}$ in a bimodal grain structure can be determined by the relation:

$$d_{geff}^{-1} = C_{CG}\, d_{gcg}^{-1} + C_{UFG} d_{gufg}^{-1}\ , \tag{15}$$

where C_{CG} is a volume fraction of coarse grains, C_{UFG} is a volume fraction of ultra fine grains, $d_{g\,cg}$ and $d_{g\,ufgf}$ are the average grain sizes of coarse and ultra fine grain fraction, respectively.

Weighted-average grain size (d_{wt}) can be defined as (Dapeng et al., 2011):

$$d_{gwt} = \sum_{i=1}^{N} d_{gi} f_{ai}\ , \tag{16}$$

where d_{gi} is the size of grain (i) and f_{ai} is the area-fraction of that grain.

Strain to failure ε_f^n at quasi static loadings increases proportionally to the inverse of the square root of the effective grain size (Lukač, 2011).

$$\varepsilon_{f\,st}^n = \varepsilon_{f\,0}^n [1 + D_{\varepsilon f} d_g^{-1/2}] / (1 - \theta), \tag{17}$$

where $\varepsilon_{f\,st}$ is the strain to fracture at quasi static loading, $\varepsilon_{f\,0}$, $D_{\varepsilon f}$ are material constants, $\theta = (T - T_r)/(T_m - T_r)$, T is the temperature, Tr =295 K, T_m is the melting temperature.

The strain to failure ε_f^n at dynamic loadings describes by relation:

$$\varepsilon_{f\,st}^n / \varepsilon_{f\,dyn}^n = [1 + C_{\varepsilon f} \lg(\dot{\varepsilon}_{eq} / \dot{\varepsilon}_0) H(\dot{\varepsilon}_{eq} / \dot{\varepsilon}_0 - 1)], \tag{18}$$

where $\varepsilon_{f\,dyn}$ is the strain to fracture under tension at high strain rate, $\dot{\varepsilon}_{eq} = [(2/3)\dot{\varepsilon}_{ij}\dot{\varepsilon}_{ij}]^{1/2}$, $\dot{\varepsilon}_0 = 1{,}0\ s^{-1}$, $C_{\varepsilon f}$ is the constant of material, H(•) is the Heaviside function.

The calculated by Eq. (18) values of strain to failure under dynamic loads for the CG and UFG aluminium alloys is shown in Fig. 4. The symbols, shown in Fig. 4, are experimental data at room temperature (Mukai, 2003).

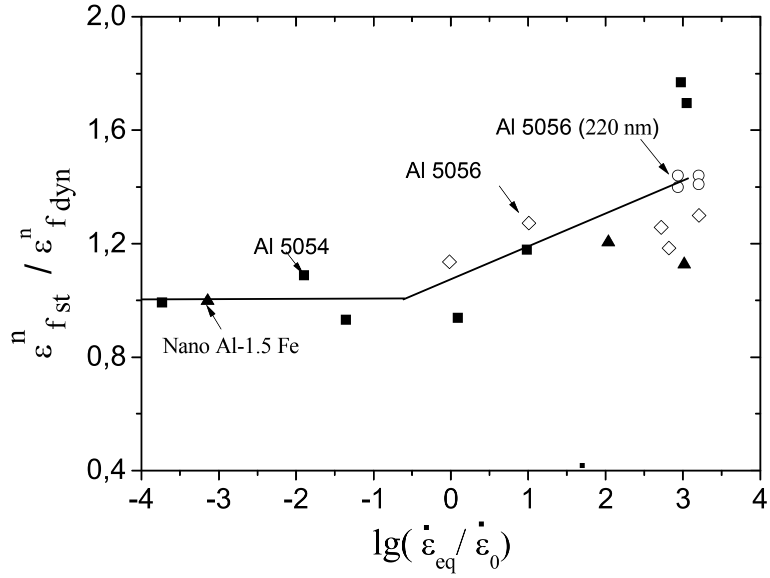

Fig. 4 - The strain to failure ε_f^n at dynamic loadings of CG and UFG aluminium alloys

The deformation to failure of UFG alloys can be determined by the relationship, taking into account the distribution of grain size:

$$\varepsilon_f^n\ (d_g)/\varepsilon_f^{CG} = A_2 + (A_1 + A_2)/(1+\exp[(d_g^{-1/2} - d_{gm}^{-1/2})/\bar{d}_g^{\ -1/2}]), \tag{19}$$

$$\varepsilon_f^{CG}\ = D_1\,(P^* + T^*)^{D_2}, \tag{20}$$

where ε_f^{CG} is the strain to fracture of coarse grained volume of material, A_1, A_2, $d_{gm,}$ $\bar{d}_g$ are the material constants, $T^*=\sigma_{sp}/p_{HEL}$, $P^*=p/p_{HEL}$, p_{HEL} is the pressure at the Hugonioy elastic limit, D_1, D_2 are the material constants.

Eq. (19) takes into account the influence of the grain size distribution on the ductility of steel (BCC crystalline structure) and FCC and HCP alloys. Universal dependence of $\varepsilon_f^n\ (d_g)/\varepsilon_f^{CG}$ on $d_g^{-1/2}$ for aluminium alloy Al 1100, magnesium alloy AZ31, and IF steel is shown in Fig.5. Symbols are shown experimental data (Han, 2004, Han, 2006, Fan, 2006, Nicaise, 2011).

The strain rate sensitivity of flow stress for UFG alloys can be defined as:

$$m = \left.\frac{d(\ln\sigma_s)}{d\ln(\dot{\varepsilon}_{eq}/\dot{\varepsilon}_0)}\right|_{T,\varepsilon^p_{eq}} = m_0 + C_m d_g^{\ -1/2}, \tag{21}$$

where σ_s is the yield strength, $\dot{\varepsilon}_{eq} = [(2/3)\dot{\varepsilon}_{ij}\dot{\varepsilon}_{ij}]^{1/2}$ is the equivalent strain rate, $\dot{\varepsilon}_0 = 1{,}0\ s^{-1}$, m_0, C_m are the material constants, d_g is the average grain size.

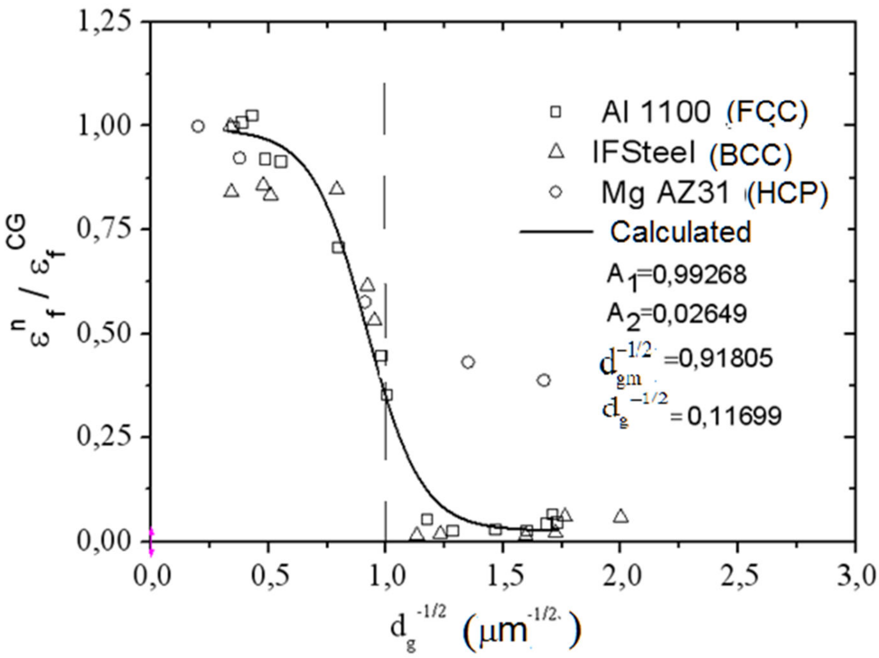

Fig. 5 - Normalized strain to fracture versus the inverse square root of effective grain size

The strain rate sensitivity of flow stress versus the inverse square root of effective grain size for FCC alloys (cooper and aluminium) and HCP magnesium alloy is shown in Fig. 6. Symbols shown in Fig. 6 are experimental data (Zhu, 2005, Skripnyak, 2014).

The model was used for numerical simulation mechanical response of model volume of alloys under tension. Calibration of the constitutive equation is performed using the original data of the authors obtained during testing specimens of alloys under the quasi-static and high-speed tests (Kozulyn, 2015, Skripnyak N., 2015). Distribution of grains in the specimens was changed due to processing by severe plastic deformation (Moskvichev, 2016).

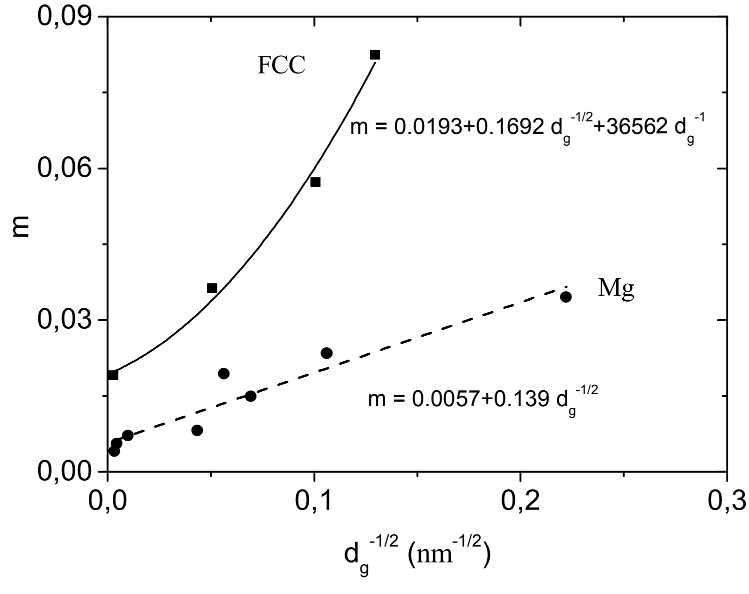

Fig. 6 - The strain rate sensitivity of flow stress versus the inverse square root of effective grain size

RESULTS

We performed a simulation of the deformation and damage of the 3D model volume of the alloy in tension at a constant speed within the range of 0.01 m/s to 15 m/s. The coarse grained and ultrafine-grained alloys were simulated in a range of strain rates from 0.1 s^{-1} to 5 10^3 s^{-1}.

The calculated stress vs strain curves of magnesium alloy MA 2-1 is shown if Fig. 7. Stress-strain curves were calculated at strain rates of 0.1 sec and a temperature of 295 K.

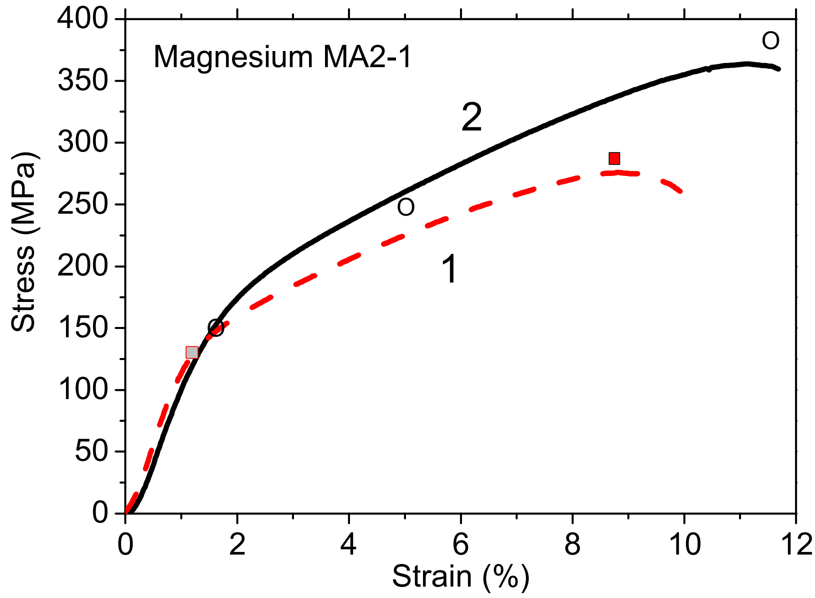

Fig. 7 - Calculated stress vs strain curves of magnesium alloy, curves (1) and (2) correspond to a unimodal and a bimodal distribution of grain size, respectively

Curve (1) was derived for unimodal grain size distribution with average grain size equal to 40 µm. Curve (2) corresponds to bimodal grain size distribution. Symbols are marked original experimental data of authors. The volume fraction of ultra fine grains was equal to ~35 %. The yield stress of the alloy increased on 10 - 15 % in comparison with a coarse-grained alloy if the volume fraction of the UFG grains is close to the percolation threshold.

Calculated dependences of the yield strength on logarithm of normalized strain rate for aluminium alloys with distribution of grain sizes are shown in Fig.8. Curves (1), (2), (3) correspond to a unimodal coarse-grained structure, unimodal fine-grained structures, and bimodal distribution of grain size, respectively. Symbols shown in Fig. 8 are experimental data (Hockauf, 2006, Meyer, 2007, Skripnyak N., 2015).

Results of numerical simulation showed that the dependences of the yield stress on logarithm of normalized strain rate for alloys with a bimodal distribution of grains and coarse-grained alloys are similar. The obtained results of numerical simulation agree with the experimental data.

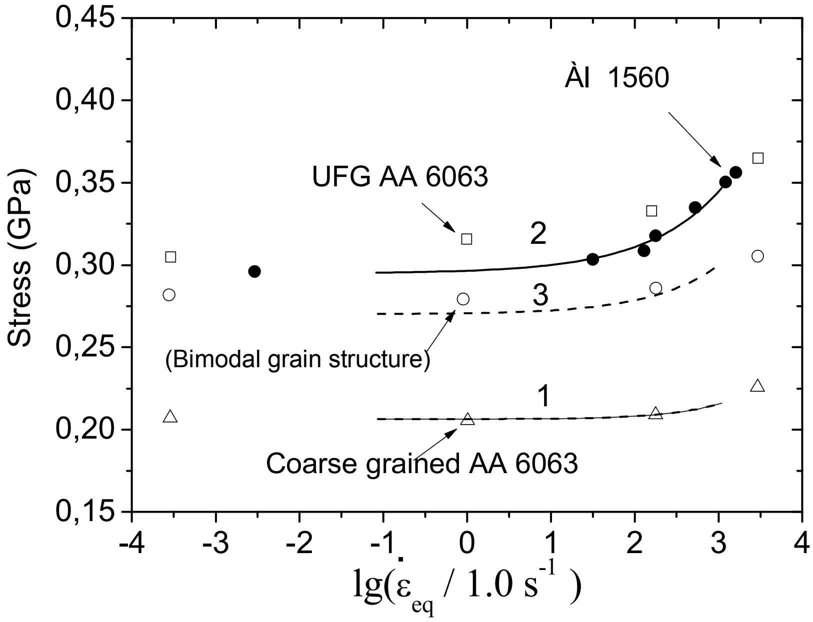

Fig. 8 - Calculated yield strength vs logarithm of normalized strain rate

CONCLUSION

The influence of grain size distribution on the mechanical behavior of magnesium and aluminium alloys in a wide range of strain rates was studied by numerical simulation method.

The model allows taking into account the distribution of grain size in HCP and FCC alloys is proposed.

The model was applied for 3D simulation of uniaxial tension of ultrafine-grained aluminium and magnesium blocks in the range of strain rate 0.1- 10^3 s^{-1}.

It was shown that the dependences of the yield stress on logarithm of normalized strain rate for alloys with a bimodal distribution of grains and coarse-grained alloys are similar.

Results of numerical simulation are shown that the yield stress of the alloy increased on 10 - 15 % in comparison with a coarse-grained alloy if the volume fraction of the UFG grains is close to the percolation threshold.

ACKNOWLEDGMENTS

This work was supported partially by the Grant from the President of Russian Federation MK-2690.2017.8, СП-1916.2015.2. The authors are grateful for the support of this research.

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