Contribution of structural factors to the deformation behaviour of nanostructured Cu-Zn alloys

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Abstract. The results of the analysis of the deformation behavior of nanostructured Cu-Zn alloys, obtained as a result of severe plastic deformation, implemented by the equal-channel angular pressing method, are presented. The role of structural factors responsible for increasing the strength characteristics and uniform elongation of the Cu-Zn alloys has been revealed.

1. Introduction

In \([1]\) it was shown that in low-carbon steels, as well as in metals with a FCC lattice at room temperature and \(\alpha\)-Ti with an HCP lattice, the true uniform elongation \(\varepsilon_u\) in the region of large grain sizes \(d\) (\(d > 10\ \mu m\)) does not depend on the grain size \(d\), while in the region of small grains the value \(\varepsilon_u\) decreases with a decrease in the value \(d\). Moreover, \(\varepsilon_u\) in alloys with a FCC lattice is higher than in alloys with a BCC lattice due to high rates of deformation hardening.

In metals in which the flow stress \(\sigma\) is sensitive to the strain rate, the strain is localized subject to the Hart criterion:

\[
\frac{1}{\sigma} \frac{\partial \sigma}{\partial \varepsilon} \leq 1 - m,
\]

\(m\) – the rate sensitivity, \(\varepsilon\) - the strain. An increase in the value of \(m\) contributes to maintaining the plasticity of the sample. Only nanostructured (NS) FCC and HCP metals have a higher rate sensitivity as compared to their coarse-grained (CG) analogues. NS BCC metals have even lower rate sensitivity \(m\) than BCC metals in the CG state \([1]\). Therefore, it is more essential to maintain high values of the strain hardening rate. It can be assumed that the nature of the dependence of \(\varepsilon_u\) on the grain size \(d\) is not due to its value, but to the dislocation microstructure formed during the deformation process. A similar relationship exists between the flow stress \(\sigma\) and \(d\). The grain size is a function of the dislocation density \(\rho_{\text{dis}}\) \([2]\). Therefore, it can be expected that there is a definite relationship between the quantities \(\varepsilon_u\) and \(\sigma\). The dependence of the value of \(\varepsilon_u\) on the true yield strength of \(Y_t\) in steels was obtained. It turned out that the value of uniform elongation is a function of the strength of the alloy: the value of true uniform elongation \(\varepsilon_u\) decreases with increasing \(Y_t\) \([1]\). Thus, the value of \(\varepsilon_u\) is determined by the state of the formed microstructure corresponding to a given grain size \(d\).

The observed differences in the deformation behavior of alloys with FCC and HCP lattices and the different strain hardening of alloys with FCC lattice can be explained by the difference in their stacking fault energy (SFE) \([3]\). It is known that alloying leads to a decrease in the SFE, an increase in
the activity of deformation twinning with a decrease in the activity of dislocation slip [4, 5]. In NS Cu and alloys of the Cu-Al system obtained by the method of equal-channel angular pressing (ECAP) [6, 7, 4], a monotonous increase in the yield stress and uniform elongation with decreasing SFE was revealed.

The purpose of this work is to analyze the role of structural factors responsible for increasing the strength and the uniform elongation of the Cu-10 wt.% Zn alloy subjected to 1 and 8 ECAP passes, as well as flat rolling (FR) after 8 ECAP passes. As a result of these alloy treatments, ultrafine-grained (UFG) states 1 ECAP, 8 ECAP and 8 ECAP+FR were formed, respectively.

2. Experimental
A detailed description of the experiments is presented in [8]. Samples of the Cu-10 wt.% Zn alloy, were kindly provided by prof. Wei Wei, Changzhou University, P.R.C., in the initial CG state and were a subject for annealing at a temperature of 1073 K for 2 h and subsequent quenching in water from a temperature of 773 K. As a result, a homogeneous structure with an average grain size of 117±50 µm was obtained (initial state - IS). The SFE of pure Cu is ~78 mJ/m², the Cu-10% Zn alloy is ~35 mJ/m². Then, the samples in the IS were subjected to 8 ECAP passes (route Bc) at a temperature of 150 °C and subsequent FR at a temperature of 150 °C to reduction degree 95%. Mechanical tensile testing of the samples was carried out on an Instron 8801 tensile testing machine at room temperature. Microstructure studies were carried out using a transmission electron microscope. Investigations of the microstructure of alloy samples subjected to ECAP revealed a significant refinement of grains, the average size of which after 1 pass was 85±5 µm, after 8 passes - 121±50 nm. Consequently, a structure with finer grains is formed in the studied alloy during the ECAP process. The average grain size after FR slightly increased and amounted to 210±60 nm. Inside the grains of the alloy in UFG states, nanotwins were observed, the volume fraction and thickness of which increased with increasing number of ECAP passes. As a result of FR after 8 ECAP passes, their volume fraction and thickness decreased. The dimensions of coherent domains D_{NQR}, the lattice parameter a, and the elastic microdistortion of the crystal lattice \( \langle \varepsilon^2 \rangle^{1/2} \) obtained by the X-ray diffraction method [9] are summarized in Table 1. The atomic fraction \( c_{Zn} \) of Zn atoms dissolved in the matrix in the UFG alloy states was calculated taking into the assumed linear dependence of lattice parameter on the concentration of Zn in solid solution. Due to the absence of the experimental lattice parameter of pure Cu, a reference value of \( a_{0}=0.3615 \) nm was used.

| The parameters of the microstructure | IS | 1ECAP | 8ECAP | 8ECAP+FR |
|-------------------------------------|----|-------|-------|----------|
| \( D_{NQR} \) (nm)                 | -  | 47±7  | 35±3  | 29±2     |
| \( \langle \varepsilon^2 \rangle^{1/2} \) (%) | -  | 0.20±0.01 | 0.31±0.02 | 0.34±0.01 |
| \( a \) (Å)                        | 3.6379±0.0001 | 3.6377±0.0005 | 3.6363±0.0007 | 3.6364±0.0005 |

3. Results and discussion
The value of dislocation density (Table 2) in various structural states of the alloy was estimated taking into account the experimental data presented in Table 1 and the values of the Burgers vector equal to \( b=a\sqrt{2}/2 \) nm according to the formula \( \rho_{tot} = 2\sqrt{3} \langle \varepsilon^2 \rangle^{1/2} / D_{NQR}b \) [10]. It was assumed that the yield stress \( \sigma_Y \) of an alloy taken in the initial state is determined by the contribution of three active factors: \( \sigma_Y = \sigma_p + \sigma_d + \sigma_{dis} \) (Table 2). The Peierls stress \( \sigma_p \) was calculated according to the simplified formula \( \sigma_p = [M G / (1 - \nu)] \exp[2\pi / (1 - \nu)] \), where the Poisson coefficient is \( \nu=0.343 \), the Taylor factor is \( M=3.05 \), the shear modulus is \( G=42.1 \) GPa [11]. Solid-solution hardening \( \sigma_d \) was calculated according.
to the dependence presented in [12]: \( \sigma_c \approx MGz^{3/2}C_{Zn} / 760 \), where the parameter \( z \) is 0.55. In this case, the atomic fraction \( C_{Zn} \) of Zn atoms dissolved in the matrix was calculated according to the equation

\[
C_{Zn} = W_{Zn} \frac{\mu_{Cu}}{\mu_{Zn}} \left( \frac{W_{Zn}}{1 - W_{Zn}} + 1 \right) \left( \frac{W_{Zn}}{1 - W_{Zn} - \mu_{Cu}} + 1 \right)^{-1},
\]

\( W_{Zn} \) is the mass fraction of Zn atoms in the alloy, \( \mu_{Zn} \) and \( \mu_{Cu} \) are the relative atomic masses of Zn and Cu, respectively. In evaluating the dislocation hardening \( \sigma_{dis} = MGz\sqrt{\rho_{dis}} \) [13], the parameter \( z \) was taken equal to 0.37 [11]. The experimental value of the true yield stress \( \sigma_y \) was calculated according to the formula \( \sigma_y = Y(1+\varepsilon_Y) \), where \( \varepsilon_Y \) - experimental value of deformation corresponding to stress \( Y \) (table 3).

With an increase in the number of ECAP passes, the dislocation density increases. This is caused by the limitation of the dislocation annihilation at their double cross-slip and climb as a result of a low SFE. At the same time, a low SFE facilitates deformation by twinning. The presence of twin boundaries contributes to the accumulation of dislocations in the inner regions of the grains.

| State  | \( \rho_{dis} \) (m\(^{-3}\)) | \( \sigma_{dis} \) (MPa) | \( \sigma_t \) (MPa) | \( \sigma_c \) (MPa) | \( \sigma_P \) (MPa) | \( \sigma_\nu \) (MPa) |
|--------|-------------------------------|--------------------------|---------------------|---------------------|---------------------|---------------------|
| IS     | 1.50 \times 10^{13}           | 47.3                     | -                   | 6.73                | 13.8                | 67.8                |
| 1ECAP  | 5.76 \times 10^{14}           | 292.8                    | 63.3                | 6.67                | 13.8                | 376.6               |
| 8ECAP  | 1.20 \times 10^{15}           | 422.7                    | 65.8                | 6.26                | 13.8                | 508.6               |
| 8ECAP+FR | 1.59 \times 10^{15}         | 486.6                    | 31.0                | 6.28                | 13.8                | 537.7               |

Table 2. Model values of dislocation density, strengthening factors and model value of yield strength \( \sigma_\nu \) of Cu-10 wt.% Zn alloy.

| State  | \( Y \) (MPa) | \( \varepsilon_Y \) (%) | \( Y_t \) (MPa) | \( f_t \) (%) | \( t \) (nm) | \( C_{dis} \) (%) | \( N_t \) |
|--------|---------------|--------------------------|-----------------|--------------|-------------|-----------------|---------|
| IS     | 120.0         | 1.0                      | 121.2           | -            | -           | 9.74            | -       |
| 1ECAP  | 368.0         | 3.8                      | 382.0           | 2.4          | 16.0        | 9.65            | 5       |
| 8ECAP  | 500.0         | 4.5                      | 522.5           | 5.3          | 21.0        | 9.06            | 3       |
| 8ECAP+FR | 520.0        | 4.0                      | 540.8           | 0.5          | 8.0         | 9.09            | 6       |

Table 3. The values of experimental \( Y \) and true \( Y_t \) yield stress, experimental strain value \( \varepsilon_Y \), volume fraction \( f_t \) and thickness \( t \) of twins, atomic fraction \( C_{Zn} \) of Zn atoms dissolved in the matrix and the number of dislocations \( N_t \) blocked at the twin boundaries.

In the case of the alloy subjected to ECAP, in addition to the above three strengthening factors, it is necessary to take into account strengthening along the boundaries of the twins. The backpressure created by the boundaries of the twins was calculated according to the formula \( \sigma_r = K_nz^{-1} \), where \( K_n = MGzN/2 \), \( z \) is the distance between neighboring twins, \( z^{-1} = f_t / \left[ 2t - f_t \right] \). The number of dislocations blocked at the boundaries of the twins \( N_t \) (table 3) was calculated taking into account the known experimental value of the true yield stress \( Y_t \) and known values of the contributions of the active hardening factors \( \sigma_{dis} \), \( \sigma_t \), and \( \sigma_P \) (table 2). With an increase in the number of ECAP passes, no saturation of the dislocation density is observed. The experimental value of the uniform elongation increases from 4% to 6% after 1 and 8 ECAP passes, respectively.

The subsequent FR of the samples after 8 ECAP passes leads to a further increase in the dislocation density (table 2), which was calculated taking into account the experimental data presented in table 1. The experimental value of uniform elongation took the value of 8.6%. The yield stress also increased (table 3). The number of dislocations \( N_t \) blocked at the twin boundaries, calculated taking into account the experimental value of the true yield strength \( Y_t \) and the calculated values of the strengthening factors \( \sigma_{dis} \), \( \sigma_t \), and \( \sigma_P \), turned out to be larger than in the states after ECAP (table 3). At the same time, the contribution of hardening by the boundaries of the twins was smaller due to a decrease in the volume fraction of twins (table 2). A decrease in the thickness and volume fraction of twins gave an
opportunity for further propagation of dislocations. There is an opportunity for further propagation and annihilation of dislocations. In this state, dislocation glide is an even more active deformation mechanism than in 8ECAP state.

4. Conclusions

The assumption was confirmed that the nature of the dependence of the uniform elongation of the Cu-10% Zn alloy on the grain size \(d\) is due to the microstructure formed during the deformation process. According to the results of the analysis, the boundaries of the twins, which appear in the process of ECAP in the Cu-10 wt% Zn alloy, increase their strength. An increase in the strain hardening of the samples of the alloy is realized as a result of the accumulation of dislocations in the inner regions of the grains in front of the twin boundaries, the volume fraction of which increases with decreasing grain size \(d\). At the same time, a low SFE limits the annihilation of dislocations during their double cross-slip, as well as the annihilation of dislocations during their non-conservative motion. An increase in strain hardening is accompanied by an increase in the uniform elongation. Additional flat rolling with the reduction degree 95% after 8 passes ECAP leads to the decrease in the volume fraction of the twins, an increase in the grain size. It can be assumed that this occurs as a result of the injection of sufficient energy into the system during the flat rolling process, which leads to a change in the morphology of the grain. Their appearance resembles pancakes elongated in rolling direction. At the same time, the dislocation mechanism of deformation is activated, the dislocation density increases, and the strain hardening increases, accompanied by an increase in the degree of uniform elongation at room temperature.

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