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## A microstructure-based model for describing the material properties of Al-Zn alloys during high pressure torsion

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### ABSTRACT

In this work, super saturated solid solution Al-30wt%Zn alloy was subjected to High Pressure Torsion (HPT). The material properties and microstructural evolution were experimentally studied. Despite strong grain refinement during HPT, the process of softening is observed. Such a material behavior is captured by a proposed model (MBWG) that takes into consideration the effects of solid solution hardening, Orowan looping and evolution of the dislocation density. Namely, the softening process occurred during HPT is attributed to decomposition of super saturated solid solution and evolution of the dislocation mean free path with plastic strain. Our simulation shows that the proposed model describes well the softening and saturation processes, and the decomposition of solid solution plays a significant role during the HPT process.

**Keywords:** Al-Zn alloys, Grain refinement, High Pressure Torsion, Modeling, Precipitates, Solid solution hardening

**Outline****1 Introduction****2 Experimental details****3 Experimental results**

3.1 Material properties

3.2 Microstructural evolution

3.3 Grain size and lattice parameter measurements

**4 Microstructure-based model (MBWG)**

4.1 Precipitation hardening

4.2 Dislocation hardening

4.3 Solid solution hardening

**5 Discussion****6 Conclusions**

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## 1. INTRODUCTION

Several techniques of severe plastic deformation (SPD) such as equal channel extrusion, asymmetric rolling and high pressure torsion (HPT) have been developed to improve the mechanical properties of metals (Segal, 1995; Valiev et al., 2000; Valiev and Langdon, 2006; Khan and Meredith, 2010; Meredith and Khan, 2012; Seipp et al., 2012). Among these techniques, HPT is especially effective to introduce extremely large shear strain due to the occurrence of strong grain refinement (Valiev and Alexandrov, 1999; Zhilyaev et al., 2003; Zhilyaev and Langdon, 2008). The HPT process has been the subject of many investigations as a new method of processing for nanostructured materials due to its ability to develop homogeneous nanostructures with high-angle grain boundaries (Valiev et al., 2003; An et al., 2010). The effect of HPT on the mechanical behavior and alterations of microstructural features have been investigated extensively for a wide range of pure and alloyed metals (Islamgaliev et al., 1997; Mishra et al., 1998; Zhilyaev et al., 2001; Zhilyaev et al., 2003; Sakai et al., 2005; Zhilyaev et al., 2005; Lugo et al., 2008; Edalati et al., 2008, 2009; Todaka et al., 2008; Ito and Horita, 2009; Edalati et al., 2011; Edalati and Horita, 2011; Ni et al., 2011; Srinivasarao et al., 2013). The previous investigations have shown that the application of HPT to aluminum-based alloys leads to both a small grain size and a high level of microhardness (Wang et al., 1996; Stolyarov et al., 1997; Islamgaliev et al., 2001; Gubicza et al., 2007, Loucif et al., 2010; Valiev et al., 2010; Zhang et al., 2010; Ghosh et al., 2012; Tugcu et al., 2012; Sabirov et al., 2013). In the work of Islamgaliev et al. (2001), nanostructured Al-Zn-Cu-Mg-Zr alloys after HPT demonstrated tensile strengths (up to 800 MPa). Y. Harai et al. (2009) and C. Xu et al. (2007) have investigated the evolution of the mechanical behavior for pure aluminum

during the HPT process. The results show that the hardness of pure Al initially increases with increasing strain, and then, after reaching a maximum value, decreases to a constant level. Xu et al. (2007) attributed an unusual softening phenomenon at large strain to easy cross-slip and dynamic recovery due to a large stacking fault energy (SFE) of Al.

Despite the large quantity of studies that have been carried out on HPT, most of them are only dedicated to microstructural evolution and mechanical characterization (Zhilyaev and Langdon, 2008). However, in the past few years, many researchers have attempted to develop various dislocation models to describe microstructural evolutions under large imposed strains (Langlois and Berveiller, 2003; Khan et al., 2006; Khan and Farrokh, 2006; Beyerlein and Tomé, 2007; Mayama et al., 2007; Farrokh and Khan, 2009; Groh et al., 2009; Starink et al., 2009; Austin and McDowell, 2011; Li and Soh, 2012; Ostapovets et al., 2012; Oppedal et al., 2012; Aoyagi et al., 2013; Bertin et al., 2013; Hansen et al., 2013; Kitayama et al., 2013; Lee et al., 2013; Wen et al., 2013). In the physically-based model developed by Starink et al. (2013), it was possible to predict the increment of hardness and grain refinement of pure metals during the HPT process. This model takes into account dislocation and grain boundary strengthening by incorporating the volume-averaged thermally activated dislocation annihilation and the grain boundary formation.

The most common models of grain refinement due to large strain, particularly under HPT, are usually based on the notion that the dislocation cell structure, which forms in the early stage of plastic deformation, gradually transforms to a fine grain structure. This type of models are based on the approach of Kocks and Mecking (2003), which describes the deformation behavior of metals and alloys in terms of a single internal

variable, namely, the total dislocation density. Estrin et al. (1998) proposed a constitutive model that describes the hardening behavior of cell-forming crystalline materials at large strains. This model considers the evolution of the dislocation densities in the cell walls and the cell interiors. Zhang et al. (2011) developed a microstructural model that is based on the evolution of geometrically necessary dislocations and statistically stored dislocations that incorporate grain refinement. A key element of this model is the assumption that, at the very high strains developed in HPT, the dislocation density reaches a saturation value.

In a previous work (Mazilkin et al., 2012), it was shown that HPT of Al-30wt%Zn alloy induces a strong grain refinement. Surprisingly, the corresponding material behavior consists in a continuous strain softening. Strain softening is usually found during hot working as a result of dynamic recovery and dynamic recrystallization. However, at room temperature, occurrences of softening were recently reported in metals subjected to SPD and were attributed to the occurrence of concomitant phenomena such as dynamic recovery, dynamic recrystallization, high-angle grain boundary development and supersaturated solid solution decomposition (Mazilkin et al., 2012). However, the existing models have not been able to connect the flow stress with the observed microstructure evolution.

In a previous work, Borodachenkova et al. (2013) made an attempt to develop a new microstructure-based model to explain the softening during HPT. The model consisted in two main components: (i) In the first stage of plastic deformation, the material behavior is dictated by the gradual increase of the dislocation mean free path resulting from precipitation, and diffusion of Zn atoms towards the grain boundary; (ii) In the second stage, further grain refinement to nanoscale size promotes a dramatic increase

in strain rate due to the diffusion-driven grain-boundary sliding according to the theory of Raj and Ashby (1971). However, with this model, the contribution of different strengthening mechanisms was not evaluated.

The purpose of this paper is to explain with a microstructure-based model the evolution of the critical resolved shear stress with the accumulated shear strain during the HPT process. This model takes into account the contribution of different strengthening mechanisms such as dislocation multiplication, Orowan and solid solution hardening. The model is based on the understanding of microstructural evolution and the interaction of dislocations with the microstructure essential features.

## 2. EXPERIMENTAL DETAILS

Al-30wt%Zn alloy was prepared by induction melting in vacuum from high purity elements (5N Al and 5N5 Zn). After melting, the alloy was poured in vacuum into a water-cooled copper crucible with an internal diameter of 10 mm. Samples of the alloy were cut by spark machining in the disks with a thickness of about 1mm and diameter of 10mm, and then polished mechanically to a thickness of 0.38 mm. The principle of HPT is described in several articles (Vorhauer and Pippan, 2004; Horita and Langdon, 2005; Zhilyaev et al., 2005). The HPT process was conducted under quasi-constrained conditions. Fig. 1 illustrates the schematic of quasi-constrained HPT, where the outer flow of the disk-shaped sample nearby its peripheries is limited.

A disk-shaped sample placed in the depression between massive anvils and is subjected to torsional straining under a high hydrostatic pressure of the order of several GPa. The HPT process in this work was performed at room temperature and conducted under an applied pressure,  $P$ , of 6.0 GPa for 0.2, 0.5, 0.7 and 1 anvil revolutions at a constant angular velocity of 1 rpm. During the processing, the main

volume of the material is deformed in conditions of quasi-hydrostatic compression.

As a result, in spite of the large strain values, the deformed sample is not destroyed.

The HPT equipment allows the direct measurement of the applied torque. The shear stress was then calculated using the following relation:

$$\tau = \frac{1}{M_\tau} \frac{3Q}{2\pi r^3} \quad (1)$$

where  $Q$  is the measured torque.  $r$  is the radius of the sample.  $M_\tau$  is the Taylor factor for torsion whose value is suggested to be 1.65 for FCC metals (Zehetbauer et al., 2004).

The shear strain of the disk subjected to HPT,  $\gamma$ , was calculated as:

$$\gamma = 2\pi RN/h \quad (2)$$

where  $N$  is the number of rotations,  $R$  the distance from the center of the sample and  $h$  the thickness of the disk (Estrin et al., 2008).

The Von Mises strain could be calculated as follow:

$$e_{eq} = \frac{\gamma}{\sqrt{3}} = \frac{2\pi RN}{h\sqrt{3}} \quad (3)$$

However, in this work, the axial strain was not considered.

All samples for structural investigations were cut from the deformed disks at a distance of 2.5 mm from the sample center. Transmission electron microscopy (TEM) investigations were carried out using a JEM-4000FX microscope operating at 400 kV. The TEM samples were prepared by electrochemical polishing. X-ray diffraction analysis (XRDA) was used to investigate the phase composition using a SIEMENS-



500 diffractometer ( $\text{CuK}\alpha_1$  radiation). The precision X-ray reflection angle in a range of  $2\theta > 100^\circ$  is used to determine the lattice parameters of the alloys by the Nelson-Riley procedure (Nelson and Riley, 1945).

The dislocation density was measured using X-ray diffraction line profile analysis. The conventional Multiple Whole Profile (MWP) fitting procedure, which is described in detail the work of Ungár et al. (2001), is used to evaluate the diffraction peak profiles. The procedure was used to estimate the density of dislocations ( $\rho$ ).

Hardness measurements were performed also at 2.5 mm from the center, using a nanoindenter (MTS Nano Instruments, Inc., Oak Ridge, TN). The system has load and displacement resolutions of 50 nN and 0.01 nm, respectively.

### **3. EXPERIMENTAL RESULTS**

#### **3.1 Material properties**

The experimental shear stress-shear strain curve of the Al-30wt%Zn alloy measured during the HPT processes is illustrated in Fig. 2. After a short positive strain hardening regime (up to 1.3), strain softening was detected until 26 plastic shear strain, after which a steady state is observed. The experimental shear stress values have been compared with hardness measurements (Fig. 3) carried out at different strain levels and a good qualitative agreement was observed.

#### **3.2 Microstructural evolution**

The microstructural evolution of Al-30wt%Zn obtained by TEM is shown in Fig. 4. This figure shows that the alloy contains Al and Zn grains with average sizes of 15 and 1  $\mu\text{m}$ , respectively (Fig. 4a). The Zn grains decorate the Al grain boundaries and present an ellipsoid shape. In the first stage of deformation (until the shear strain of

10.5), a strong precipitation of Zn occurs in the bulk and at the Al grain boundaries. In addition, the pinned dislocations self-organized structures give rise to highly misoriented grain boundaries (new grains) (Fig. 4b). With increasing strain, the Zn precipitates grow in size (from about 20 to 60 nm) and the Zn atoms diffuse and reform grain boundary precipitates (Fig 4c, 4d). At a shear strain of 52 (Fig. 4e), the bulk of Al grains is almost free of precipitates and dislocations, which indicates that intensive recovery has occurred.

TEM observations suggest that dislocations in the bulk of Al and grain boundaries serve as nucleation sites for Zn precipitates. Before the deformation, the concentration of Zn atoms inside the solid solution is very high. With increasing deformation, the dislocations rearrange and self-organize to form new grain boundaries which become heavily enriched in Zn. The dislocations pinned at precipitates contribute to Zn redistribution by pipe diffusion. In addition, the intense pinning produces an effective division of the grains leading to sub-grain boundaries, which contribute to an even higher rate of solute diffusion towards the growing precipitates. In this way, Zn concentration in Al decreases due to dislocation motion into the sub-grain boundaries, which controls the softening process. It is well known that the grain boundary and pipe diffusions are much faster than the bulk diffusion for solute. The schematic view of the grain refinement for Al-Zn alloys during HPT processes is presented in Fig. 5.

### 3.3 Grain size and lattice parameter measurements

The evolution of the grain size with shear strain for Al and Zn grains is illustrated in Fig. 6. After shear strain up to 10.5, the grain sizes of Al and Zn decrease, respectively to 1.2  $\mu\text{m}$  and 0.43  $\mu\text{m}$ . Further deformation resulted in grain refinement down to 0.55  $\mu\text{m}$  after shear strain of 36.5.

It is well-known that in a super saturated solid solution Al-Zn alloy, the lattice parameter of aluminum is strongly influenced by Zn atoms. The XRDA of Al-Zn alloys before and after HPT shows that it contains two phases, namely (Al) solid solution and (Zn) solid solution grains. According to the equilibrium phase diagram, the Al-Zn alloys contain two phases at room temperature: (Al) solid solution with Zn content less than 0.5 wt% and (Zn) solid solution with Al content less than 0.1 wt%. Due to the intensive occurrence of precipitation during HPT, the lattice parameter of Al should also increase during the process. The values of the lattice parameter for Al-based solid solution at different shear strains are listed in Table 1. It can be seen that the lattice parameter increases until a shear strain of 26 (value close to that of pure Al). In our case, the supersaturated solid solution with an initial concentration of 17 wt% decomposes completely after shear strain of 26.

#### 4. MICROSTRUCTURE-BASED MODEL (MBWG)

According to the previous observation, it is assumed that the total strength of Al-Zn alloy is expressed as

$$\tau - \tau_{ss} = \tau_{dis} + \tau_{Orowan} \quad (4)$$

where  $\tau_{ss}$ ,  $\tau_{dis}$  and  $\tau_{Orowan}$  are the strengthening related with solid solution, dislocation density and Orowan mechanism, respectively.

##### 4.1 Precipitation hardening

The importance of  $\tau_{Orowan}$  was well illustrated by the microstructural analysis revealing that during the first steps of plastic deformation (until shear strain of 10.5), Al grains contain a population of small Zn-rich precipitates, which were assumed to

impede the motion of dislocations. In the present approach,  $\tau_{Orowan}$  is supposed to depend on both the Zn precipitate inter-spacing ( $\omega$ ) and their size ( $d$ ) according to the following expression (Kocks, 1966; Gubicza et al., 2007):

$$\tau_{Orowan} = k_{or} \frac{0.85\mu b \ln\left(\frac{d}{b}\right)}{2\pi(\omega - d)} \quad (5)$$

According to the experimental measurement, the Zn precipitates grow in size (from about 20 to 60 nm); the distance between precipitates also evolves between 300 nm and 600 nm.  $k_{or}$  is introduced in Eq. (5) to describe approximately  $\tau_{Orowan}$  evolution for the initial step of the deformation and to eliminate its contribution after the shear strain of 10.5. In fact, the strong Zn precipitation only occurs in the bulk of Al grains at the beginning of the plastic deformation. In this work,  $k_{or}$  is imposed to be increased linearly from 0 to 1 until the shear strain of 1.3, and then decreased linearly to 0 until the shear strain of 10.5.

#### 4.2 Dislocation hardening

The contribution of dislocation hardening is assumed to depend on the average dislocation density (the same in every grain) through the usual Taylor law:

$$\tau_{dis} = \alpha\mu b\sqrt{\rho} \quad (6)$$

where  $\alpha$  is a dislocation-dislocation interaction coefficient,  $\mu$  the elastic shear modulus,  $b$  the Burgers vector and  $\rho$  the dislocation density.

In the approach proposed by Kocks and Mecking (2003), the annihilation process is thermally activated and governed by the glide of dislocations at low and medium

temperature regimes. Thus, the evolution of the dislocation density with shear strain is given by:

$$\frac{d\rho}{d\gamma} = \frac{1}{bL} - f\rho - k_e\rho \quad (7)$$

where  $k_e = (d_e/d)^2$  as defined by Li and Soh (2012).  $d_e$  is a reference grain size corresponding to the critical grain size at which enhanced dynamic recovery occurs, and  $d$  is the grain size. The critical grain size for Al alloy is around 1  $\mu\text{m}$  (Hariprasad et al., 1996).  $L$  is the dislocation mean free path and  $f$  a recovery term.

In the present formulation,  $L$  is considered as an independent state variable that evolves with shear deformation as shown in Eq. (8).

$$\frac{dL}{d\gamma} = d_{sat}e^{-m\gamma} - d_r e^{-n\gamma} \quad (8)$$

where  $d_{sat}$  is the saturation grain size.  $m$  and  $n$  are the balance parameters.  $d_r$  identifies the representative distance between Zn precipitates during the HPT processes which is approximately calculated by  $d_r = \frac{L_{max} + \omega_i}{2}$  in this work.  $\omega_i$  and  $L_{max}$  are respectively the initial and maximum Zn precipitate interspacing during the HPT processes.

Unlike in the Kocks-Mecking original approach, here the mean free path is first assumed to be determined by the precipitate interspacing and, after some amount of plastic deformation, by the refined grain size.. Indeed, as discussed in the next section,  $L$  should be significantly lower than the mean free path of the original Kocks-Mecking model, which is controlled by dislocation interspacing and grain size. The

two terms on the right side of Eq. (8) characterize two of the main physical processes involved in the plastic deformation process: Orowan looping controlled by the distance between precipitates and the saturation grain size.

Integration of Eq. (8) leads to the following expression for  $L$  :

$$L = \int \frac{dL}{d\gamma} = \int d_{sat} e^{-m\gamma} - \int d_r e^{-n\gamma} = -\frac{d_{sat}}{m} e^{-m\gamma} + \frac{d_r}{n} e^{-n\gamma} + c_i \quad (9)$$

where  $c_i$  is an integration constant. According to the microstructural observations, it is clear that when  $\gamma \rightarrow \infty$ ,  $L \rightarrow d_{sat}$ , and therefore  $c_i = d_{sat}$ . Under this circumstance we obtain:

$$L = -\frac{d_{sat}}{m} e^{-m\gamma} + \frac{d_r}{n} e^{-n\gamma} + d_{sat} \quad (10)$$

### 4.3 Solid solution hardening

It is well-known that solid solution strengthening is related with the interactions of gliding dislocations with solute atoms and is highly sensitivity to the temperature. In order to describe such an effect, Kocks and Mecking (1981) proposed a model based on a thermally activated stress component. In the present work, a modified version of this approach is introduced which is dependent on the Zn atom concentration in Al and a thermal component as proposed in the original version.

$$\tau_{ss} = k_l \left[ \tau_0 + a_0(c) \left[ 1 - \left( \frac{kT}{\Delta G} \ln \frac{\dot{\gamma}_0}{\dot{\gamma}} \right)^{2/3} \right] \right] \quad (11)$$

where  $\tau_0$  is the friction stress,  $k$  the Boltzmann constant,  $T$  the temperature,  $\Delta G$  the activation energy for deformation.  $\dot{\gamma}_0$  is the characteristic strain rate which is related

to the vibrational frequency of dislocations arrested at an obstacle or, alternatively, the attempt frequency for overcoming an obstacle (Kocks et al., 1975).  $k_f$  is introduced in Eq. (11) to approximately describe the evolution of  $\tau_{ss}$  for the initial step of deformation. This parameter is imposed to be linear increasing from 0 to 1 at the beginning of the deformation, and remain to be 1 during the softening process.  $a_0$  is the value of thermal stress at 0 K dependent on the Zn concentration in Al grains ( $c$ ). An expression of  $a_0$  is proposed based on the analysis of Zaiser (2002) and Olmsted et al., (2006):

$$a_0 = \tau_p + \frac{3A}{2b^3} \left( \frac{\sqrt{2}\hat{U}^4}{A\omega_0} \right)^{1/3} \sqrt{c} \quad (12)$$

where  $\tau_p$  is the Peierls stress,  $\hat{U}$  the characteristic interaction energy between a single solute and a straight dislocation,  $A$  an adjustable scaling factor,  $\omega_0$  the characteristic range for the interaction, and  $A$  the line tension energy per unit length of dislocation which can be expressed as (Soare and Curtin, 2008):

$$A = \frac{3\mu b^2}{4\pi(1-\nu)} \quad (13)$$

here  $\nu$  is the Poisson ratio.

Based on the lattice parameter measurements and the relationship between this parameter and Zn concentration in Al grain investigated in the work of Ellwood (1952), the intensity of solid solution decomposition was evaluated by determining the evolution of Zn concentration in Al during HPT. The concentration evolution was described as:

$$c = c_1 \exp(-c_2 \gamma) - c_3 \exp(-c_4 \gamma) + c_{sat} \quad (14)$$

where  $c_1$ ,  $c_2$ ,  $c_3$  and  $c_4$  are modeling parameters, and  $c_{sat}$  is the equilibrium Zn concentration in Al grains.

## 5. Discussion

In order to calculate the dislocation mean free path  $L$ , the coefficients  $m$  and  $n$  in Eq. (8) need to be determined. For that, several boundary conditions should be introduced. First, based on TEM observations (Fig. 4), it was possible to verify that the value of  $L$  obtained for  $\gamma = \gamma_1 \approx 10.5$  is about 600 nm ( $L_{max}$ ). Such a condition can be expressed by:

$$-\frac{d_{sat}}{m} e^{-m\gamma} + \frac{d_r}{n} e^{-n\gamma} + d_{sat} = L_{max} \quad (15)$$

Second, when  $\gamma = 0$ , Eq. (10) becomes:

$$-\frac{d_{sat}}{m} + \frac{d_r}{n} + d_{sat} = \omega_1 \quad (16)$$

Eqs. (15, 16) enable the calculation of the parameters  $m$  and  $n$  in Eq. (8) which are listed in Table 2. Then, the evolution of  $L$  with plastic strain is shown in Fig. 7. By considering the evolution of  $L$  and integrating Eq. (7), the dislocation density is obtained as a function of the plastic strain (see Fig. 8). It can be seen that the dislocation density increases at the beginning of the plastic deformation, then decreases dramatically until a shear strain around 10.5 and finally keeps a steady value. Due to the intense annihilation process verified at the beginning of HPT, an



unusual high recovery parameter  $f$  of 6330 has to be considered to get a good approximation between model and experiment.

As mentioned in section 4, the Kocks-Mecking model suppose that  $L$  is determined by the dislocation interspacing and the grain size, whereas the MBWG model assumes that the evolution of  $L$  is due to the precipitate interspacing, and the refined grain size after certain plastic deformation. In this case, the  $L$  calculated by the MBWG model should be much lower than the one of Kocks-Mecking model. To validate this point, we propose a comparison of  $L$  determined by both models. According to the Kocks and Mecking approach, the dislocation mean free path is dependent on the square-root of the dislocation density and the grain size:

$$\frac{1}{L_{K-M}} = \frac{\sqrt{\rho}}{K} + \frac{1}{D} \quad (17)$$

with  $K$  the number of forest dislocations a moving segment is able to cross before being trapped by the obstacles.  $D$  is the initial grain size of Al. In the present work, the exact value of  $K$  for Al-30wt%Zn alloy cannot be obtained. Therefore, we select several values of  $K$  between the minimum value ( $K = 1$ ) and the value of  $K = 30$  which is suggested for AA 6022-T4 by literature (Rauch et al., 2007). The calculated mean free paths with Eqs. (8) and (17) are shown in Fig. 9.. However, we can notice that, for all the  $K$  values, the mean free path calculated with the Kocks-Mecking approach is much larger than that obtained with the MBWG model. This suggests that during HPT of Al-Zn alloys, the dislocation mean free path is mainly controlled by the density of precipitates, and then, by the refined grain size. In contrast, the dislocation density has a minor effect on the mean free path.

The evolution of  $\tau_{dis}$  with shear strain shown in Fig. 10 is calculated according to Eq. (6). It can be seen that such a low dislocation density produces a maximum  $\tau_{dis}$  around 3 MPa. This means that the dislocation density strengthening mechanism does not play a significant role during HPT process of Al-Zn alloy.

In the calculation of Zn concentration in Al, the parameters in Eq. (14), which is listed in Table 2, is adjusted according to experimental results. The simulated and experimental Zn concentrations are shown in Fig. 11. Based on this, the evolution of the solid solution stress can be calculated by Eqs. (11-14). In those equations, the Peierls stress is suggested to be  $\tau_p \approx 3$  MPa (Soare and Curtin, 2006). In the analysis of Olmsted et al. (2006) for Al-Mg alloys, the value of  $\hat{U}$  and  $A$  have been determined to be around 0.1 eV and 2, respectively, and  $\omega_0$  belongs to the range between 10~20 Å. In the present work, the value of  $\hat{U}$  and  $\omega_0$  are adapted for Al-Zn alloys by a fitting process, and all the parameters in Eqs. (11-14) are listed in Table 2. The calculated evolution of  $\tau_{ss}$  is presented in Fig. 12. Comparison of the contribution of the hardening mechanisms is presented in Fig. 13. We should note that the values of  $\tau_{ss}$  is much higher than  $\tau_{dis}$  and  $\tau_{Orowan}$ .

On the basis of the previous analysis, it is possible to calculate the stress-strain curves using Eq. (4). The curve predicted by the MBWG model is presented and compared with experimental result in Fig. 14. It can be seen that the MBWG model describes well both the softening and saturation processes during HPT. Moreover, the calculation indicates that the softening process is mostly associated with a strong decrease of  $\tau_{ss}$  due to the depletion of Zn atom solutes in the Al grains.

## 6. CONCLUSIONS

In the present work, the material properties of Al-30wt%Zn alloy deformed under High Pressure Torsion (HPT) have been studied. It has been shown that HPT leads to a strong softening process at the beginning of plastic deformation. The material properties have been compared with the microstructural evolution. It has been shown that the fundamental phenomena of the process are solid solution decomposition, Orowan looping and dislocation density, respectively. The material properties are dictated at the beginning of plastic deformation by the decomposition of supersaturated solid solution and after saturation strain by saturation grain size.

The softening process has been well captured with a new model called MBWG that is based on strain induced diffusivity of Zn in Al grains and the evolution of the dislocation mean free path with plastic strain. The model considers the material properties to be determined by the gradual increase in the mean free path of dislocations resulting from precipitation and diffusion of Zn atoms towards the grain boundaries.

The calculated results by MBWG model present a good agreement with experiment. This model shows the capability to describe both the softening and saturation processes. The calculated shear stress evolution is mostly contributed by the solid solution shear stress. This suggests that the decomposition of super saturated solid solution plays the dominated role in the material properties of Al-30wt%Zn alloy. The MBWG model allows evaluate the contribution of the different strengthening mechanisms during the deformation and it can be adapted to other softening processes during plastic deformation.

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## FIGURE CAPTIONS

Fig. 1. Schematic illustration of quasi-constrained HPT setup

Fig. 2. Experimental shear stress-shear strain curve obtained during HPT process

Fig. 3. The hardness measurements at different strain level

Fig. 4. The microstructural evolution of Al-30wt%Zn during HPT, for the initial state (a) and at different strain level: (b)-  $\gamma = 10.5$ , (c)-  $\gamma = 26$ , (d)-  $\gamma = 36.5$  and (e)-  $\gamma = 52$

Fig. 5. Schematic view of grain refinement of Al-Zn alloys during HPT process.

Fig. 6. The evolution of the grain size with shear strain

Fig. 7. The calculated evolution of the dislocation mean free path with shear strain

Fig. 8. The experimental and calculated evolutions of the dislocation density with shear strain

Fig. 9. The comparison of the evolution of dislocation mean free path with shear strain calculated by the approach of Kocks and Mecking (Eq. 17) and MBWG model (Eq. 8)

Fig. 10. The calculated evolution of the  $\tau_{dis}$  shear stress with shear strain

Fig. 11. The evolution of Zn concentration in Al grains with shear strain

Fig. 12. The calculated evolution of  $\tau_{ss}$  shear stress with shear strain

Fig. 13. The comparison of the contribution of different hardening mechanisms

Fig. 14. Comparison between the predicted and experimental shear strain-shear stress curves.

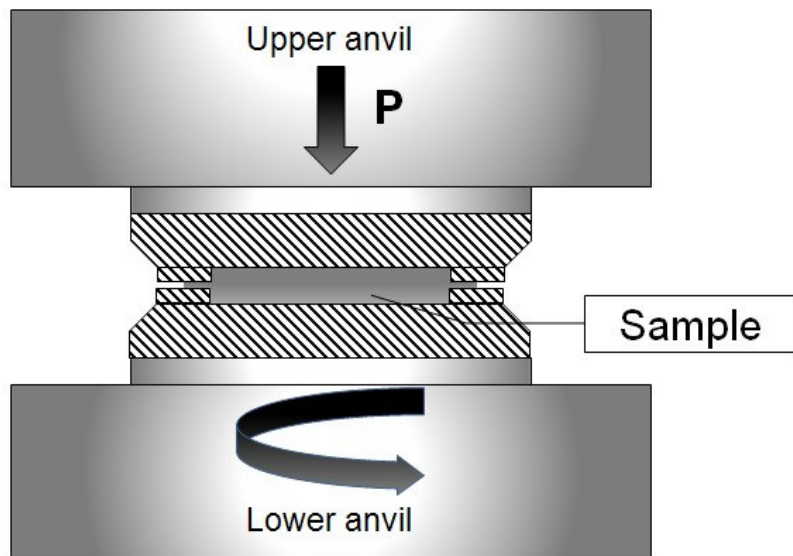


Fig. 1. Schematic illustration of quasi-constrained HPT setup

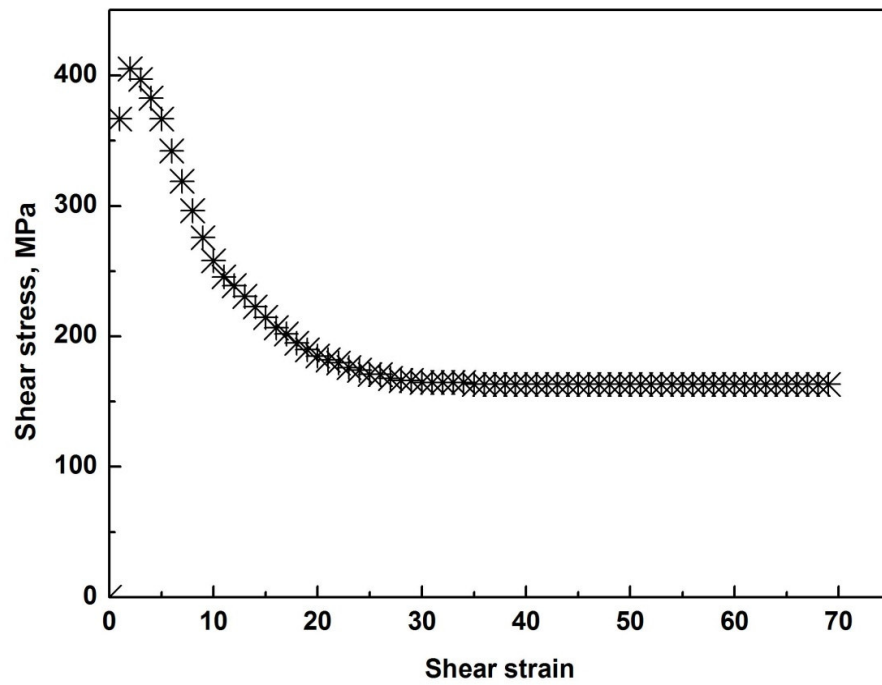


Fig. 2. Experimental shear stress-shear strain curve obtained during HPT process

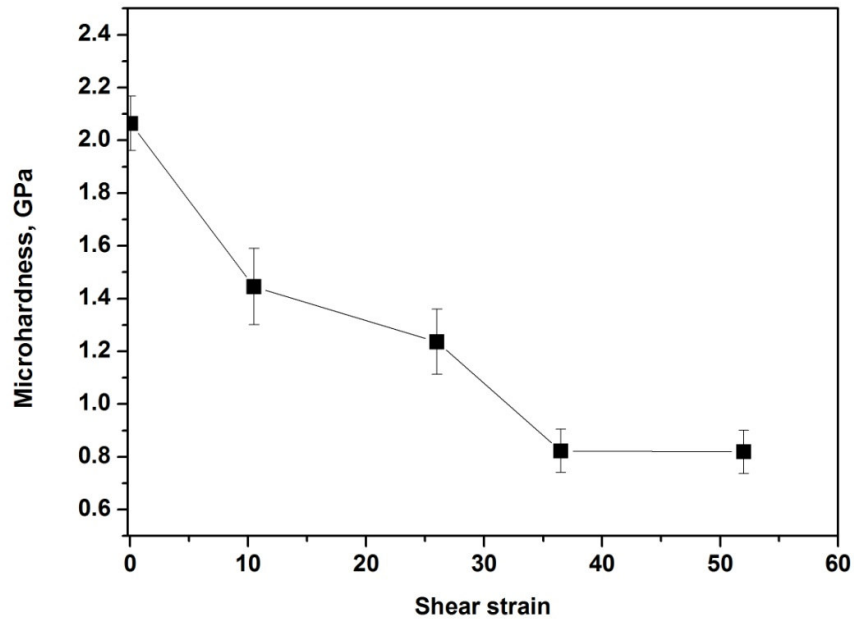
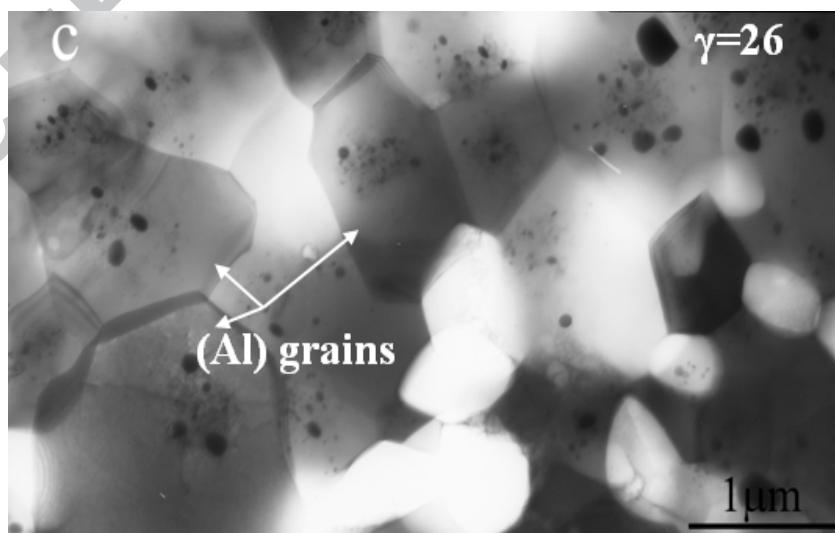
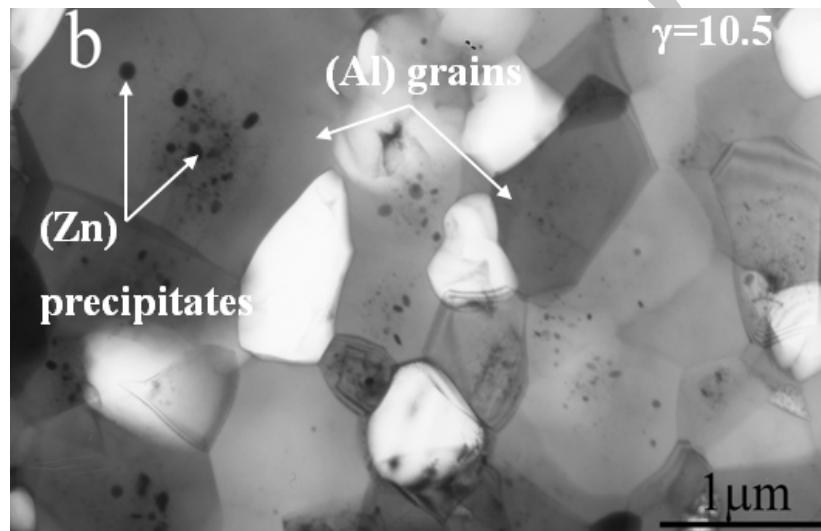
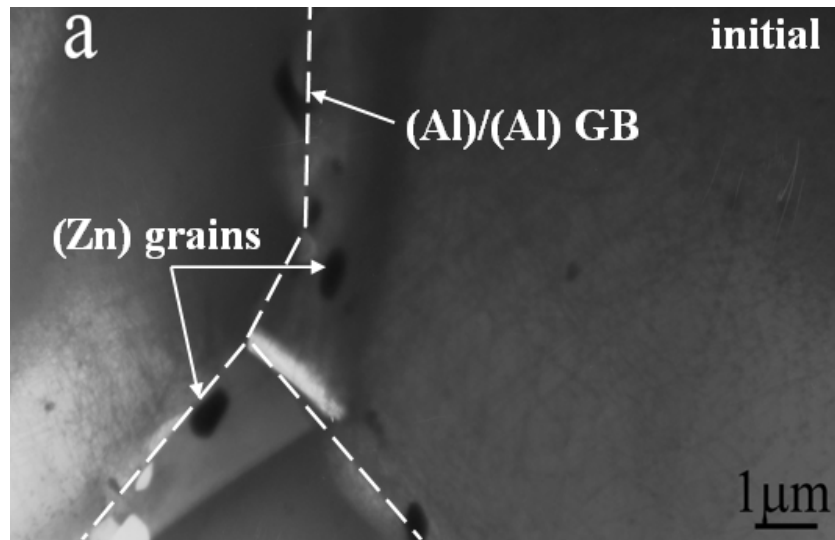


Fig. 3. The hardness measurements at different strain level



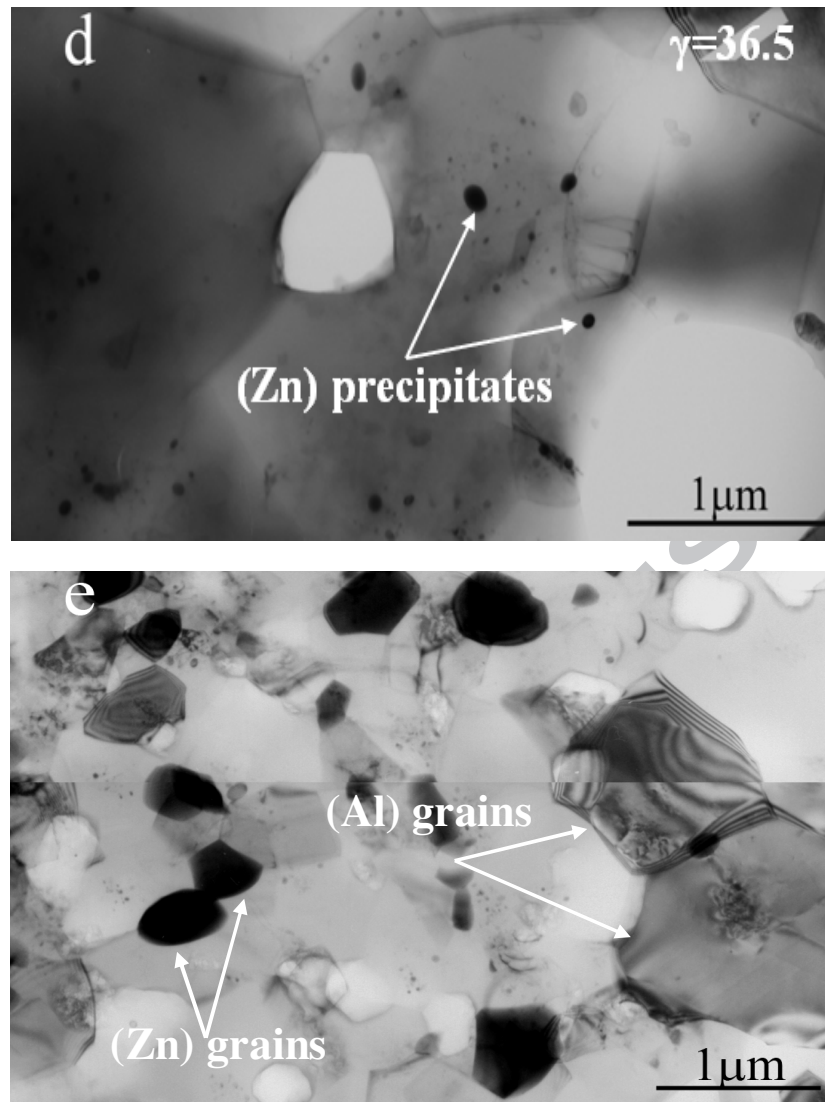


Fig. 4. The microstructural evolution of Al-30wt%Zn during HPT, for the initial state (a) and at different strain level: (b)- $\gamma = 10.5$ , (c)-  $\gamma = 26$ , (d)- $\gamma = 36.5$  and (e)- $\gamma = 52$

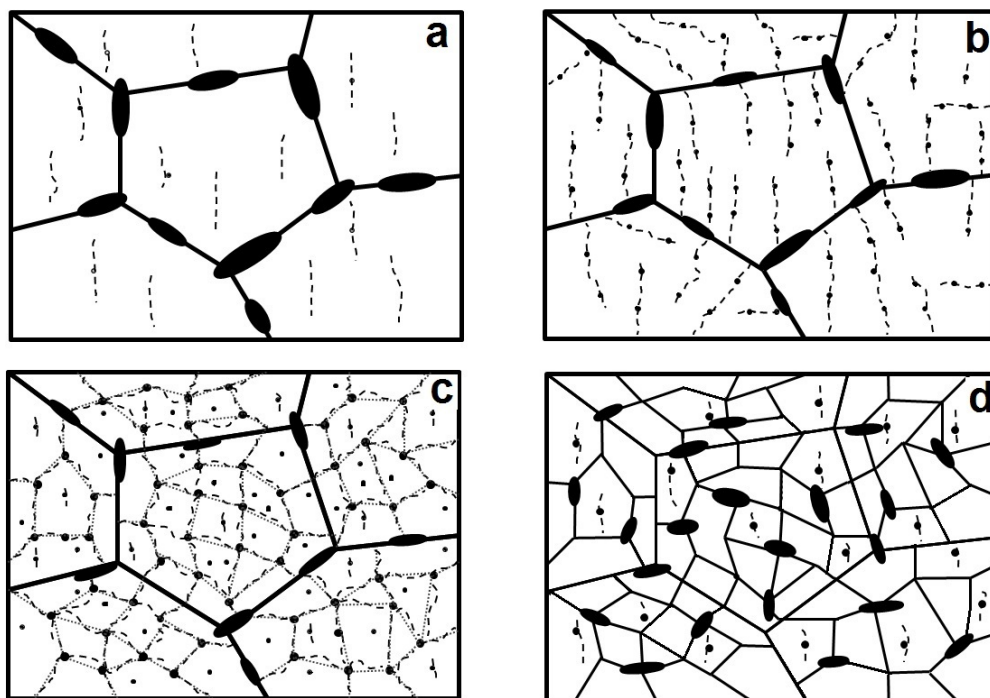


Fig. 5. Schematic view of grain refinement of Al-Zn alloys during HPT process. In this sketch the large black ellipses indicate Zn grains located at the grain boundaries, while the smaller black circles indicate Zn precipitates within the grain. The black dash lines indicate dislocations pinned by precipitates and forming regular arrays in the grains, while the gray lines in Fig. 5c illustrate the division of grains into sub-grains. The continuous lines in Fig. 5d demonstrate the new grains after refinement.



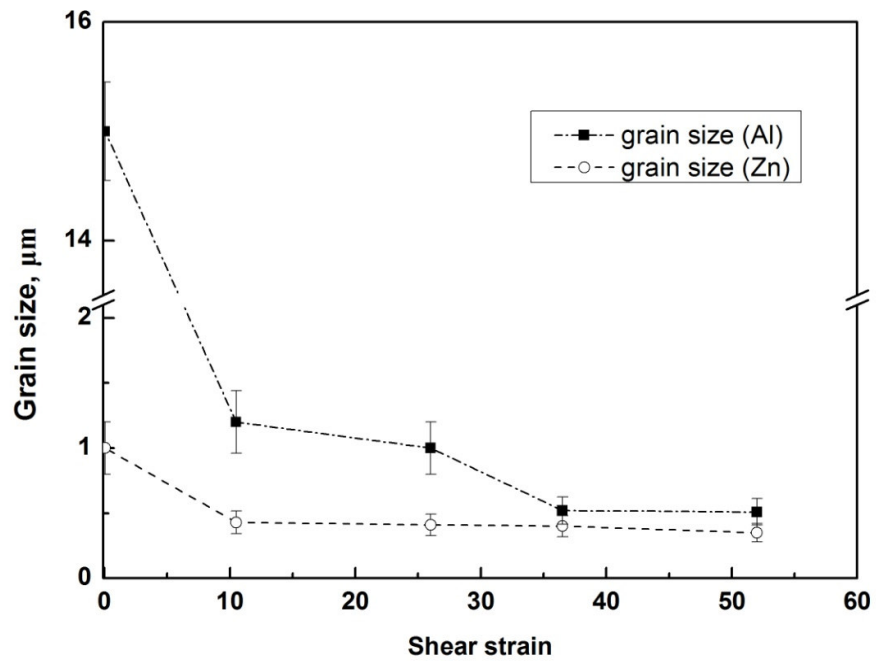


Fig. 6. The evolution of the grain size with shear strain

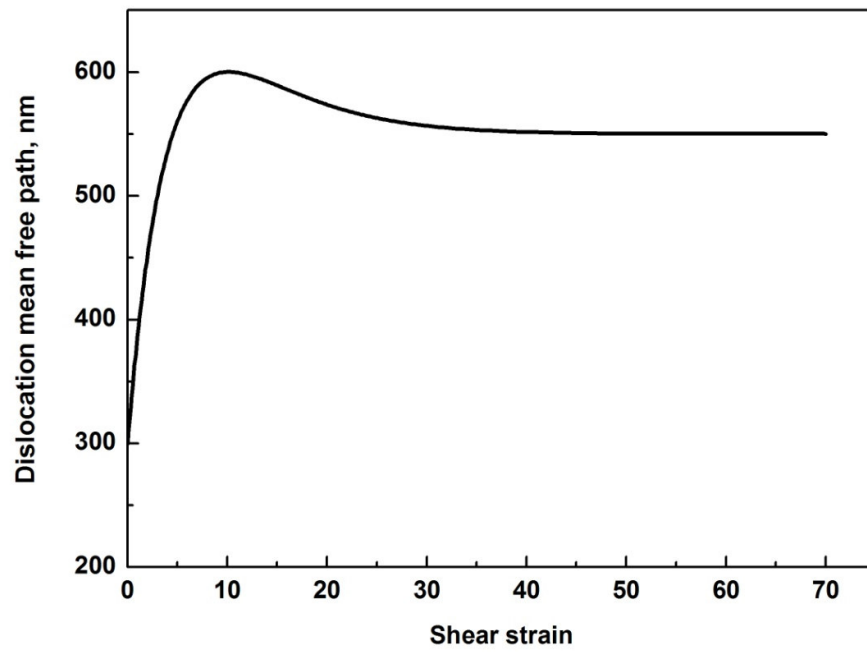


Fig. 7. The calculated evolution of the dislocation mean free path with shear strain

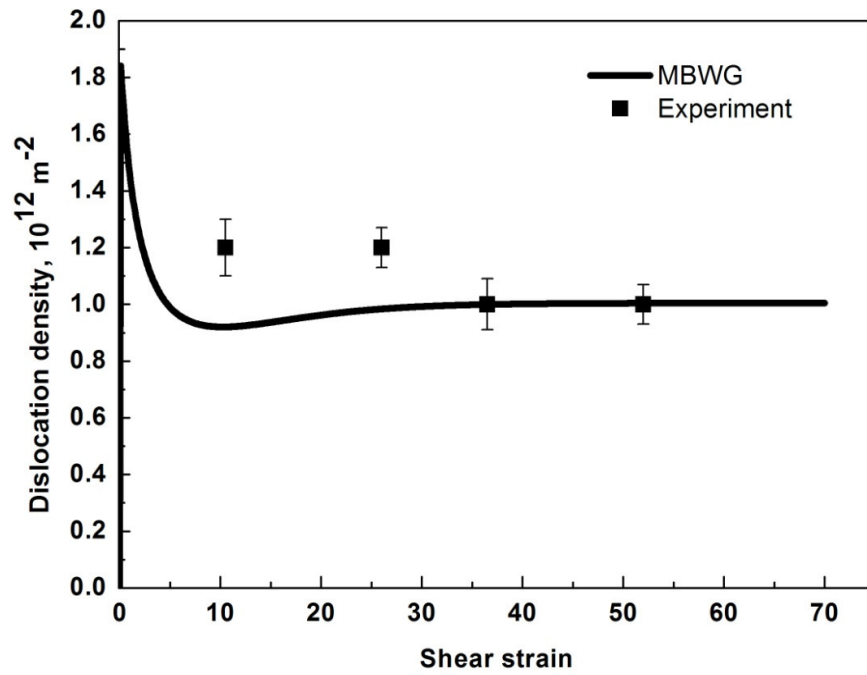


Fig. 8. The experimental and calculated evolutions of the dislocation density with shear strain

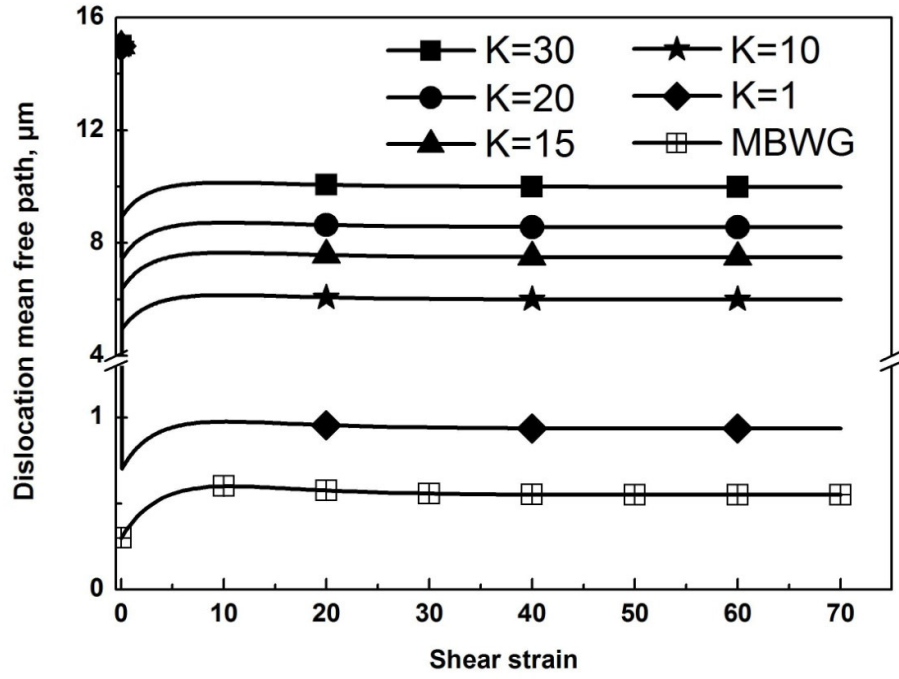


Fig. 9. The comparison of the evolution of dislocation mean free path with shear strain calculated by the approach of Kocks and Mecking (Eq. 17) and MBWG model (Eq. 8)

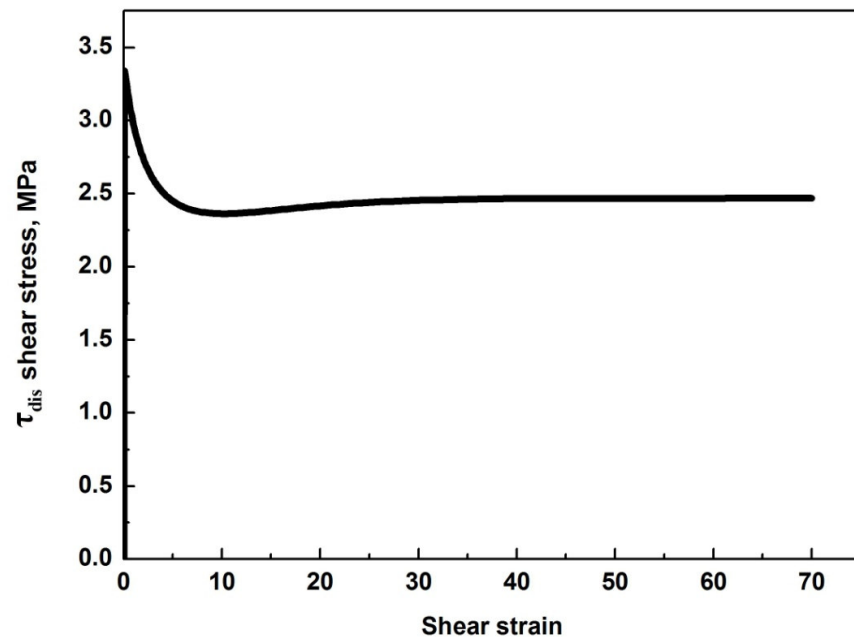


Fig. 10. The calculated evolution of the  $\tau_{dis}$  shear stress with shear strain

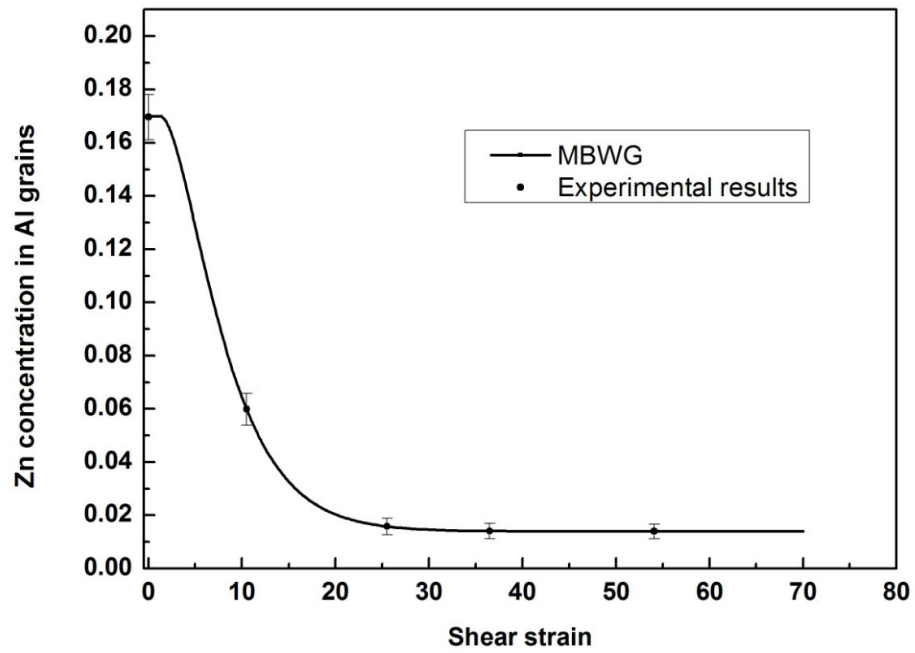


Fig. 11. The evolution of Zn concentration in Al grains with shear strain

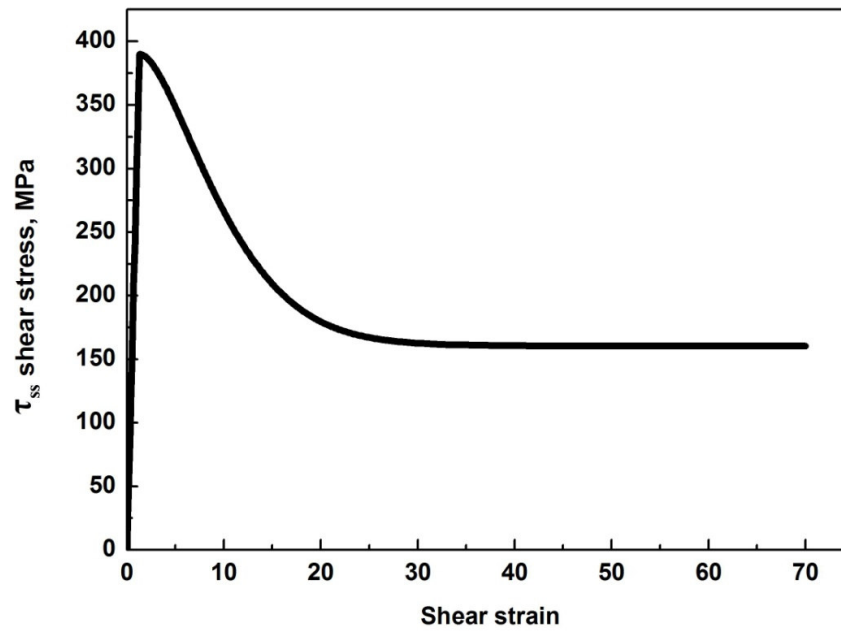


Fig. 12. The calculated evolution of  $\tau_{ss}$  shear stress with shear strain

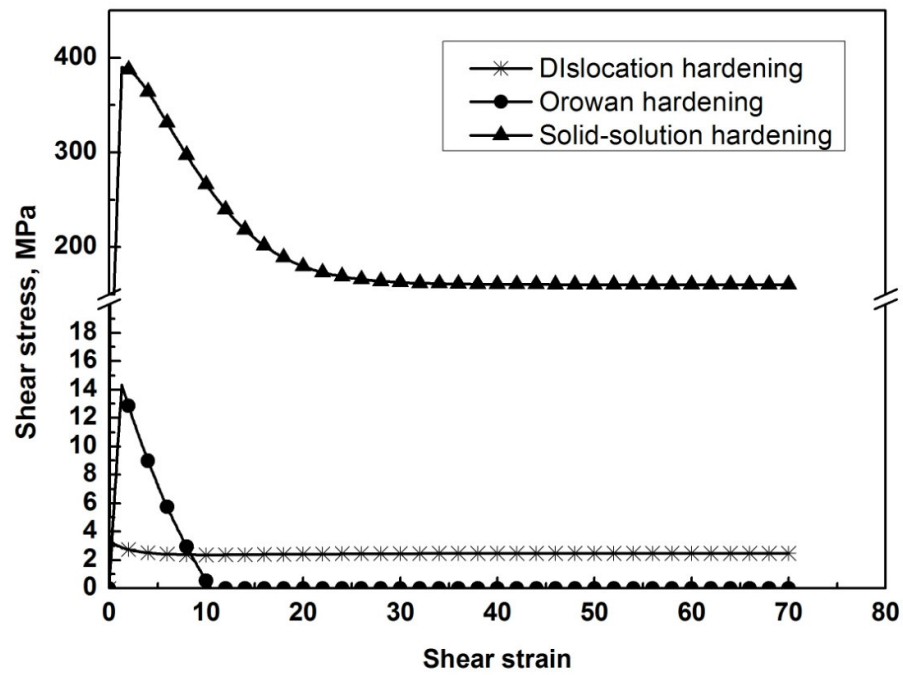


Fig. 13. The comparison of the contribution of different hardening mechanisms



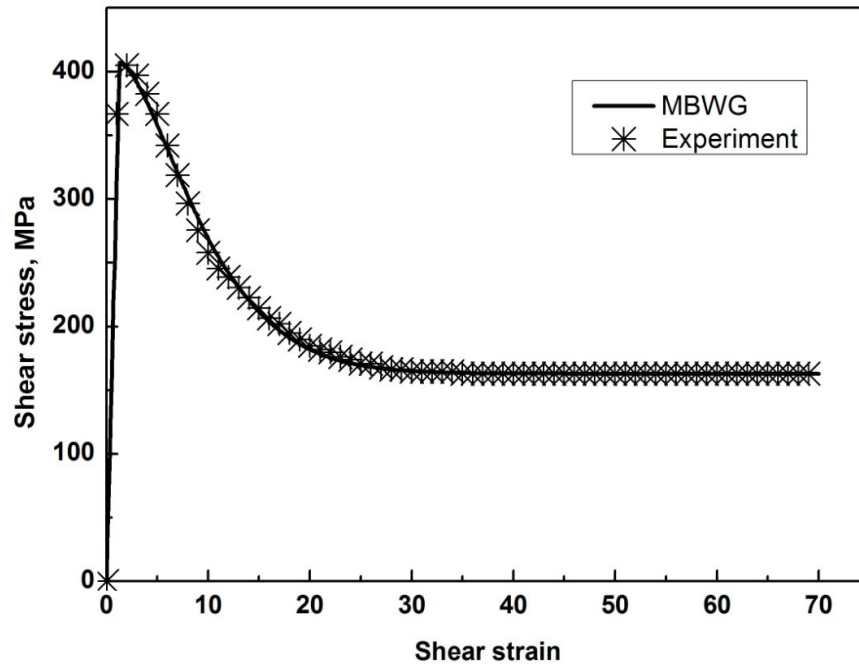


Fig. 14. Comparison between the predicted and experimental shear strain-shear stress curves.

shear strain	lattice parameter, nm
initial	0.40437±0.000023
10.5	0.40471±0.00003
26	0.40485±0.00003
36.5	0.40485±0.00003
52	0.40485±0.00003

Table 1. Lattice parameter of Al-30%wtZn alloy for different shear strains during

HPT

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	Al-30%wtZn
$\mu$ (elastic shear modulus)	26 GPa
$b$ (Burgers vector)	0.287 nm
$\alpha$ (dislocation-dislocation interaction)	0.33
$\tau_0$ (friction stress)	65 MPa
$\omega_1$ (initial distance between Zn precipitates)	300 nm
$L_{max}$ (maximum distance between Zn precipitates)	600 nm
$d_1$ (initial size of Zn precipitates)	20 nm
$f$ (dynamic recovery term)	6330
$\rho_0$ (initial dislocation density)	0
$\rho_{sat}$ (saturation dislocation density)	$10^{12} \text{ m}^{-2}$
$c_1$ (constant)	1.15
$c_2$ (constant)	0.242
$c_3$ (constant)	1.005
$c_4$ (constant)	0.2964
$c_{sat}$ (equilibrium Zn concentration in Al grains)	0.014
$m$ (constant)	0.189
$n$ (constant)	0.169
$d_e$ (critical grain size)	1 $\mu\text{m}$
$d_{sat}$ (saturation grain size)	550 nm
$\gamma_{sat}$	26
$\Delta G$ (activation energy for dislocations interactions with the solute structures)	2 eV
$\dot{\gamma}_0$ (characteristic strain rate)	$10^7 \text{ s}^{-1}$
$\dot{\gamma}$ (shear strain rate)	$0.867 \text{ s}^{-1}$
$T$ (temperature)	298 K
$k$ (Boltzmann constant)	$1.38 \times 10^{-23} \text{ J/K}$
$\tau_p$ (Peierls stress)	3 MPa
$A$ (adjustable scaling factor)	2
$\hat{U}$ (characteristic interaction energy between a single solute and a straight dislocation)	0.162 eV
$\omega_0$ (characteristic range for the interaction)	10 $\text{\AA}$

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$\nu$ (Poisson ratio)	0.347
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Table 2. The parameters of the model

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**Highlights**

- The softening process of Al-30wt%Zn alloy during High Pressure Torsion (HPT)
- Development of a new microstructure-based model (MBWG)
- Effect of the solid solution decomposition, Orowan looping and dislocation density
- Observation of the strong grain refinement during HPT
- Simulation of the softening and saturation processes of Al-Zn alloy during HPT

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