Post-print of a Model for the Effect of Grain Size on Ductility in Ultrafine-grained Steel

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Abstract

Based on the dislocation pile-up model previously proposed by the authors and incorporating the relationship between fracture strength and grain size, a calculation model was established for the critical grain size at which grain refinement leads to reduced total elongation in ultrafine-grained steel. Using the example of grain size reduction from 10 mm to 0.2 mm, the calculation results show that the total plastic elongation of steel initially increases with decreasing grain size; however, when the grain size is reduced to approximately 2.5 mm, the total elongation of steel not only ceases to increase but also exhibits a significant decrease with further grain refinement. This result is in good agreement with recent experimental observations in ultrafine-grained materials research. The present study demonstrates that the primary mechanism causing the reduction in elongation of ultrafine-grained steel is that when grain refinement reaches a certain extent, the resistance of grain boundaries to dislocation source activation increases, leading to a significant reduction in the number of mobile dislocations, which in turn causes a substantial decrease in strain.

Full Text

Preamble

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MODEL OF THE EFFECT OF GRAIN SIZE ON PLASTICITY IN ULTRA-FINE GRAIN SIZE STEELS

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Abstract

Based on our earlier preliminary work, a model was developed for prediction of the critical grain size where plasticity would decrease as grain refinement proceeds. In the model, the effect of grain size on fracture strength was incorporated. The prediction of the model exhibited that, taking the grain size range of 10 mm to 0.2 mm as an example, the total elongation of steels would initially increase. However, when the grain size was refined to 2.5 mm and below, the total elongation of steels not only ceased to increase but decreased sharply, which shows good agreement with experimental results published recently. The present work illustrates that the dominant mechanism for the decreased elongation in ultra-fine grain size materials is the increased resistance force of grain boundaries on dislocation sources, resulting in difficulty in activating dislocation movements. Its manifestation is the decrease of plastic strain at the macroscopic level.

KEY WORDS plasticity, ultrafine grain size, grain size, dislocation pile-up, dislocation source

Introduction

The key technology for achieving strengthening and toughening of high-grade pipeline steel is the use of thermal mechanical control processing (TMCP) to refine grains, ensuring that pipeline steel obtains good low-temperature toughness at high strength levels to meet service requirements for impact fatigue during oil and gas transportation in arctic and other extremely cold regions [1,2]. However, pipeline routes inevitably pass through geologically harsh areas. To ensure that pipeline steel does not fracture due to deformation caused by geological changes during extreme conditions such as earthquakes or landslides, which could lead to oil and gas leakage and secondary damage, pipeline steel must possess not only satisfactory strength and toughness but also good capacity to withstand plastic deformation [3,4].

Numerous studies [5–9] have demonstrated that when grain size is refined to a certain range, the conventional materials science principle that material plasticity increases with grain refinement no longer applies to most ultra-fine grain steels. Experimental results [5-9] show that when grains are refined beyond a critical value, steel plasticity decreases rapidly with further grain size reduction, and the work hardening capacity is lost, thereby greatly reducing the deformation capability of steel. Therefore, reasonable microstructural design is needed to improve the plastic deformation capacity of pipeline steel—requiring grain refinement to ensure sufficient strength and toughness on one hand, while ensuring that such refinement does not cause plasticity reduction on the other. To achieve this goal, systematic analysis of the influence 规律 and mechanism of grain size on steel plastic deformation behavior is necessary, along with determination of the corresponding critical grain size, to provide a technical foundation for the design and production of new-generation pipeline steel.

Current explanations for the experimental phenomenon of plasticity decrease with grain size reduction fall into two main categories: (1) significant dynamic recovery in ultra-fine grain steel acts as a softening mechanism, reducing the work hardening rate [5,10,11]; and (2) plastic instability occurs early in deformation in ultra-fine grain steel, limiting uniform elongation to very low levels [11,12]. However, these studies have focused primarily on nanoscale materials [13] and computational research [14,15]. Systematic analysis and in-depth investigation of the microscopic physical mechanism underlying this plasticity decrease with grain size reduction in submicron-scale ultra-fine grain steel are still lacking, and no quantitative analysis model has been reported for the "critical grain size" at which plasticity begins to decrease rapidly with grain refinement in ultra-fine grain steel. This creates difficulties in microstructural design for optimizing pipeline steel mechanical properties through grain size control in actual production.

Although our previous work proposed using a dislocation pile-up model [16] as a basis for analyzing the effect of grain size on strain, the analysis foundation only addressed material deformation behavior under certain applied stress conditions without considering the effect of grain size on strength. The present work combines the influence of grain size on the fracture strength of ultra-fine grain steel and utilizes a dislocation motion model to analyze the effect of grain size on the total plastic elongation during tensile deformation of ultra-fine grain steel. Using X80 pipeline steel as an example, the critical grain size at which plastic deformation during tension transitions from increasing to rapidly decreasing with grain refinement was calculated.

1. Model for the Relationship Between Material Fracture Strength and Grain Size

The total plastic elongation of a material is the strain at fracture strength and reflects the material' s plastic deformation capability to some extent. Since changes in grain size cause variations in fracture strength, analyzing the effect of grain size on plasticity requires first examining the effect of grain size on fracture strength. Based on Stroh' s model [17], Smith [18] proposed a model for crack nucleation and propagation in metallic materials. According to Smith' s model, the critical applied shear stress for stable existence of microcracks in adjacent grains is expressed as [18]:

$$\tau = \sqrt{\frac{2E\gamma_s}{\pi(1-\nu^2)d}}$$

where τ represents the critical shear stress for stable existence of microcracks in adjacent grains, i.e., the critical shear stress for crack propagation through grain boundaries and onset of unstable propagation; E is the elastic modulus; ν is Poisson' s ratio; γ_s is the effective surface energy; and d is the grain size.

Research [18–21] has shown that for polycrystalline plastic materials, the main factor determining fracture strength is crack propagation along grain boundaries, meaning that grain boundaries are effective barriers to crack propagation [21]. In other words, even if a crack propagates through a carbide/ferrite interface, if the stress cannot overcome the "ferrite grain strength," the crack will stop at the first ferrite/ferrite grain boundary it encounters. According to Curry and King [22], the "ferrite grain strength" is given by Eq. (1). For polycrystalline materials, since each grain has a different crystallographic orientation, the resolved shear stress on slip systems of differently oriented grains under the same applied stress varies. The softest-oriented grain with the maximum orientation factor experiences the maximum resolved shear stress on its slip system. Therefore, as applied stress increases, the resolved shear stress on the slip system of the softest-oriented grain reaches τ first. When the resolved shear stress on the slip system of one grain reaches τ, microcracks begin to propagate plastically and unstably in the polycrystalline material, even if the resolved shear stress on slip systems of other grains has not yet reached τ. Thus, the fracture strength σ_f of polycrystalline materials can be expressed as:

$$\sigma_f = \frac{\tau}{m_{\max}} = \frac{1}{m_{\max}}\sqrt{\frac{2E\gamma_s}{\pi(1-\nu^2)d}}$$

where σ_f is the fracture strength of polycrystalline materials and $m_{\max}$ is the orientation factor of the softest-oriented grain in the polycrystalline material. Theoretically, the maximum possible orientation factor for a grain is 0.5 [23].

Using X80 pipeline steel as an example for calculation, the parameters E = 208 GPa [24], $\nu = 0.273$ [25], $\gamma_s = 2.6$ J/m^2 [26], and $m_{\max} = 0.5$ [23] were substituted into Eqs. (1) and (2). The relationship between σ_f and d was obtained, as shown in Figure 1 [Figure 1: see original paper]. It can be seen that σ_f increases with decreasing d, particularly when $d > 4 \sim 5$ mm, σ_f increases significantly with decreasing d. When $d < 4 \sim 5$ mm, σ_f increases more slowly with decreasing d. This is because grain boundaries can alter crack propagation paths and effectively hinder crack propagation. The smaller the d, the more grain boundaries exist, the more grain boundaries the crack encounters during propagation, the more tortuous the crack path, and the more obstacles it must overcome, thus requiring more energy for crack propagation [27]. On the other hand, finer grains result in shorter dislocation pile-up groups, fewer dislocations in the pile-up, and smaller stress concentration, making crack nucleation and propagation more difficult [23].

2. Calculation of Total Plastic Elongation

2.1 Calculation of Average Orientation Factor

The macroscopic mechanical properties of polycrystalline materials represent the average behavior of numerous grains. In actual polycrystalline materials, each grain has a different crystallographic orientation. Therefore, when the macroscopic tensile stress equals σ_f, the resolved shear stress on slip systems of individual grains differs. To discuss the relationship between total plastic elongation and d in polycrystalline materials, the relationship between σ_f and the resolved shear stress on slip systems of individual grains must first be analyzed.

At fracture, the relationship between σ_f and the resolved shear stress on a grain' s slip system is given by [28]:

$$\tau_i = \sigma_f m_i$$

where τ_i is the resolved shear stress on the slip system of the ith grain under external force, and m_i is the orientation factor of the ith grain, expressed as [29]:

$$m_i = \cos\phi_i \cos\lambda_i$$

where ϕ_i is the angle between the external stress axis and the slip plane normal, and λ_i is the angle between the external stress axis and the slip direction.

Materials research typically employs the average orientation factor for calculations. Assuming polycrystalline materials have random orientation characteristics, crystallographic theory indicates there are 936 representative orientations in orientation space [29]. Therefore, orientation space can be divided into 936 micro-regions, each characterized by orientation g_i, orientation density weight $f(g_i)$, and orientation factor $m(g_i)$. The average orientation factor $\bar{m}$ of the polycrystal is [29]:

$$\bar{m} = \sum_{i=1}^{936} f(g_i) m(g_i)$$

X80 pipeline steel has a bcc structure with 24 common $\{123\}\langle 111\rangle$ slip systems. Since dislocations on $\{123\}$ slip planes can be accomplished through combinations of slip on $\{110\}$ and $\{112\}$ planes, $\{123\}\langle 111\rangle$ slip is neglected in calculations [30]. Therefore, the orientation factors for the 12 $\{110\}\langle 111\rangle$ slip systems and 12 $\{112\}\langle 111\rangle$ slip systems in the g_i orientation micro-region are [29]:

$$m_{g_i}^{\{110\}} = \cos\phi_{g_i}^{\{110\}} \cos\lambda_{g_i}^{\{110\}}$$
$$m_{g_i}^{\{112\}} = \cos\phi_{g_i}^{\{112\}} \cos\lambda_{g_i}^{\{112\}}$$

where $m_{g_i}^{\{110\}}$ is the orientation factor for $\{110\}\langle 111\rangle$ slip systems in the g_i orientation micro-region, $\phi_{g_i}^{\{110\}}$ is the angle between the external stress direction and the normal to the $\{110\}$ plane of the g_i orientation micro-region, and $\lambda_{g_i}^{\{110\}}$ is the angle between the external stress direction and the $\langle 111\rangle$ direction of the g_i orientation micro-region. $m_{g_i}^{\{112\}}$ is the orientation factor for $\{112\}\langle 111\rangle$ slip systems in the g_i orientation micro-region, $\phi_{g_i}^{\{112\}}$ is the angle between the external stress direction and the normal to the $\{112\}$ plane of the g_i orientation micro-region, and $\lambda_{g_i}^{\{112\}}$ is the angle between the external stress direction and the $\langle 111\rangle$ direction of the g_i orientation micro-region.

However, the critical resolved shear stresses for slip on $\{110\}$ and $\{112\}$ planes in the crystal are not identical. To simplify calculations, this work uses the most common ratio $\tau_y^{\{112\}}/\tau_y^{\{110\}} = 0.95$ for bcc crystals at room temperature [31,32] and normalizes by taking the maximum orientation factor after normalization. The normalized $m(g_i)$ is expressed as:

$$m(g_i) = \max\left(\frac{m_{g_i}^{\{110\}}}{m_{\max}^{\{110\}}}, \frac{0.95 m_{g_i}^{\{112\}}}{m_{\max}^{\{112\}}}\right)$$

According to Eqs. (5)-(7), the average orientation factor $\bar{m}$ of the material can be calculated. For randomly oriented materials, the calculated $\bar{m}$ is approximately 0.459.

When the applied stress reaches σ_f, only grains with the largest orientation factors actually reach the plastic deformation corresponding to σ_f, while other oriented grains have not. Using $\bar{m}$ to calculate the resolved shear stress on slip systems yields the average resolved shear stress on slip systems of all grains, which corresponds to the macroscopic plastic deformation of the polycrystalline material. When the external stress equals σ_f, the average resolved shear stress on slip systems of grains in the polycrystalline material is [29]:

$$\bar{\tau} = \sigma_f \bar{m}$$

where $\bar{\tau}$ can be considered the equivalent value of the resolved shear stress τ_i on the slip system of the ith grain in the polycrystalline material. Based on Eq. (8), the average resolved shear stress $\bar{\tau}$ on slip systems of polycrystalline materials with different grain sizes at their corresponding fracture strength can be calculated, which is then used as the applied shear stress to calculate the effect of grain size on total plastic elongation.

2.2 Relationship Between Displacement of a Single Grain and Grain Size Under Fracture Strength

As shown in Figure 2 [Figure 2: see original paper], under the action of average resolved shear stress $\bar{\tau}$, dislocation sources at grain centers are activated, dislocations glide to grain boundaries, and a dislocation pile-up group forms in front of the grain boundary [16].

According to previous research results, the relationship between the displacement of a single grain and d can be expressed as [16]:

$$D_f = b\sum_{i=1}^{N_d} x_i$$

where D_f is the displacement of a single grain at fracture strength, b is the magnitude of the Burgers vector, N_d is the total number of dislocations in the pile-up group at fracture strength, and x_i is the position of the ith dislocation in the pile-up group. N_d and x_i are calculated by [33]:

$$N_d = \frac{\pi(1-\nu)\bar{\tau}d}{Gb}$$

$$x_i = \frac{Gb}{4\pi(1-\nu)\bar{\tau}}\left[\frac{i(i+1)}{2}\right]$$

In reference [16], τ is a given applied shear stress. In reality, changes in grain size affect not only the displacement caused by dislocation slip within grains but also the material' s strength. Therefore, comparing material plastic deformation using a single given applied stress is insufficiently accurate. Consequently, this work uses the fracture strength corresponding to the grain size as the applied stress, obtains the average resolved shear stress on slip systems through calculation of the average orientation factor, and calculates the plastic deformation of grains with different sizes individually. Using X80 pipeline steel tensile plastic deformation as an example, with $G = 77.5$ GPa, $\nu = 0.273$, and $b = 0.248$ nm [25], the plastic deformation displacement achievable by grains of different sizes under their corresponding fracture strength was calculated, as shown in Figure 3 [Figure 3: see original paper].

Figure 3 shows that although σ_f increases with decreasing d, D_f under the corresponding fracture strength for each grain size still exhibits a decreasing trend with d. This indicates that although decreasing d leads to increased σ_f, the effect of d on the number of dislocations in pile-ups and dislocation slip distance is more significant than the effect of applied stress. Currently, TMCP can refine grain size in pipeline steel to below 10 mm, with the finest grain size achievable being 1-2 mm [34]. Assuming the fracture strengths at $d = 1$ mm and $d = 10$ mm (1946 MPa and 616 MPa, respectively) are used as given tensile applied stresses to calculate the relationship between D_f and d, the results show an approximately linear relationship between displacement and d under constant stress conditions, as indicated by the dashed lines in Figure 3. However, under the corresponding fracture strength, the relationship between D_f and d is no longer linear, as shown by the solid line in Figure 3. This demonstrates that when the applied stress is constant and does not change with d, the plastic deformation displacement of a single grain exhibits an approximately linear relationship with d. According to the previous analysis, when $d > 4 \sim 5$ mm, the change in σ_f with d is no longer significant. In this grain size range, the relationship between D_f and d under corresponding fracture strength can be approximated as linear. When $d < 4 \sim 5$ mm, σ_f shows a strong dependence on d, and the increase in applied stress plays a significant role in material deformation behavior. The increase in applied stress partially offsets the effect of decreasing d on D_f, making the relationship between d and D_f non-linear, as shown by the solid line in Figure 3.

2.3 Relationship Between Activation Probability of Frank-Read Sources and Grain Size Based on Fracture Strength

For a given grain size, as tensile stress increases, the number of dislocation pile-ups increases, inevitably leading to increased plastic deformation of single grains. However, as shown by the solid line in Figure 3, although σ_f increases with decreasing d, D_f still decreases. According to relevant research [16,35], the activation probability of Frank-Read (FR) sources is affected not only by the shear stress acting on the FR source but also by the ratio of FR source length to d. In ultra-fine grain steel, for a given FR source length, smaller d results in more significant obstruction by grain boundaries to dislocation multiplication from FR sources, as shown in Figure 4 [Figure 4: see original paper].

As shown in Figure 4, for a given FR source length, when grain size is large (d_a), grain boundaries exert weak obstruction to dislocation multiplication from the FR source, allowing the FR source to emit a complete stable dislocation loop. When grain size is small (d_b), the obstruction from grain boundaries becomes significant, preventing the FR source from emitting a stable dislocation loop and thus preventing its activation.

Previous work [16] has established the relationship between FR source activation probability and both d and stress in polycrystalline materials. This work incorporates the relationship with σ_f and uses the corresponding fracture strength as the applied stress. The relationship between FR source activation probability and d in polycrystalline materials can be expressed as:

$$F_f = \int_{l_{\min}}^{l_{\max}} f(l_{FR}) dl_{FR} = \int_{Gb/\tau_{\text{nuc}}}^{0.5d} f(l_{FR}) dl_{FR}$$

where F_f is the activation probability of FR sources when applied stress equals fracture strength, $f(l_{FR})$ is the log-normal distribution function of FR source lengths in polycrystalline materials, l_{FR} is the FR source length, $l_{\min}$ is the minimum FR source length that can be activated when applied stress equals fracture strength, and $l_{\max}$ is the maximum FR source length that can be activated.

Similarly, using X80 pipeline steel tensile plastic deformation as an example and considering the relationship between σ_f and d, the effect of d on F_f in polycrystals was calculated, as shown by the solid line in Figure 5 [Figure 5: see original paper]. For comparison, using the fracture strengths at $d = 1$ mm and $d = 10$ mm as given applied stresses, the relationship between F_f and d was also calculated, with results shown as dashed lines in Figure 5. All three curves show that F_f in polycrystals decreases with decreasing d, because surrounding grain boundaries restrict FR source activation—the smaller the d, the closer the FR source is to surrounding grain boundaries, and the greater the restriction. Figure 5 shows that applied stress has little effect on F_f, because the nucleation strength of most FR sources is relatively low, and the resolved shear stress on slip systems during plastic deformation is sufficient to reach the nucleation strength of FR sources. Therefore, the key factor affecting whether FR sources can be activated is grain size, i.e., the ratio of FR source length to grain size, while the effect of increased applied stress on F_f can be neglected.

2.4 Calculation Model for Total Plastic Elongation of Polycrystalline Materials

Based on our previous model [16] and comprehensively considering the relationship between fracture strength and grain size, the relationship between single grain displacement and grain size when applied stress equals the corresponding fracture strength, and the relationship between dislocation source activation probability and grain size analyzed in this work, the relationship between plastic strain at fracture and grain size in steel can be calculated as:

$$\varepsilon_f = \frac{1}{a} \times a \times n(d) \times \sum_{i=1}^{N_d} x_i \times c \times F_f = \frac{0.5 \times b \times c \times F_f}{d^2} \times \sum_{i=1}^{N_d} x_i$$

where ε_f is the plastic strain at fracture in steel; a is the length of steel in the deformation direction; $n(d)$ is the number of grains participating in plastic deformation per unit volume, which is inversely proportional to d^3 [16]; and c is the average value of the cosine of the angle between all grain slip directions and the macroscopic deformation direction in steel, which can be calculated using the method provided in reference [16].

The conversion from true strain to engineering strain at steel fracture is given by [36]:

$$e_f = \exp(\varepsilon_f) - 1$$

where e_f is the engineering strain at steel fracture, defined as the total plastic elongation, and ε_f is the true strain at steel fracture.

2.5 Model Predictions and Experimental Validation

Substituting the material parameters of X80 pipeline steel [25] into the calculation yields the relationship between e_f and d at fracture, as shown in Figure 6 [Figure 6: see original paper]. It can be seen that as d decreases from 10 mm to 0.2 mm, e_f first increases and then decreases rapidly, with the critical grain size at which e_f transitions from increasing to decreasing being approximately 2.5 mm. The calculation results show that after considering the effect of d on σ_f, the relationship between e_f and d is consistent with the trend described in reference [16]. This again demonstrates that refining grains to a certain size range can improve steel strength and toughness, but further grain refinement significantly reduces steel plasticity. Notably, after considering the effect of d on σ_f, the critical grain size at which steel plasticity transitions from increasing to decreasing with grain refinement is approximately 2.5 mm, which is closer to experimental values than the 4.24 m calculated in reference [16].

Figure 7 [Figure 7: see original paper] shows experimental data from the literature [5,6,9,37-42] for the relationship between plastic elongation and d in one IF (interstitial-free) steel, five low-carbon steels, and three TWIP (twinning-induced plasticity) steels. Although these experimental data come from different steel types prepared by various methods, they exhibit similar patterns: when $d > 1 \sim 3$ mm, steel plasticity increases with decreasing d; when $d < 1 \sim 3$ mm, steel plasticity decreases rapidly with further d reduction. The critical grain sizes indicated by these experimental data are similar, mostly concentrated in the range of 1-3 mm, where plasticity transitions from increasing to rapidly decreasing with grain refinement. The model predictions from this work agree well with experimental results, providing validation for the model.

2.6 Analysis and Discussion

The above analysis shows that e_f in steel exhibits a pattern of first increasing then rapidly decreasing with decreasing d. Therefore, to ensure steel possesses excellent strength and toughness while maintaining good plasticity, microstructural design should ensure grain refinement does not exceed the critical grain size. Using X80 pipeline steel as an example, when d decreases from 10 mm to approximately 2.5 mm, e_f increases from about 7.5% to about 25%. However, as d further decreases, e_f rapidly decreases with decreasing d. When d decreases from 2.5 mm to 0.5 mm, e_f decreases from about 25% to only about 1%, losing the effect of introducing soft ferrite phase into the hard bainite matrix to enhance plasticity. Theoretically, controlling the introduced ferrite grain size above 2.5 mm can ensure pipeline steel achieves good plasticity while maintaining excellent strength and toughness.

According to the above analysis, this decrease in e_f caused by d reduction is mainly due to the greatly reduced activation probability of dislocation sources in the material, leading to a substantial decrease in the number of actually activated dislocation sources. Using X80 pipeline steel as an example, when d decreases from 2.5 mm to 0.5 mm, F_f decreases from 2% to only 0.002%—a reduction of three orders of magnitude. Although the total number of potential dislocation sources in polycrystalline materials is enormous, when d falls below the critical grain size, the proportion of activatable dislocation sources rapidly drops to an extremely low level, causing a severe shortage of actually activatable dislocation sources in the polycrystalline material. This severely limits plastic deformation of polycrystalline materials, causing macroscopic e_f to decrease rapidly with decreasing d.

This work uses total plastic elongation at corresponding fracture strength as the parameter to measure steel plastic deformation capacity. Based on the relationship between steel fracture strength and grain size, a model for the relationship between steel plasticity and grain size during tensile plastic deformation was established. Model analysis and calculation results show that when grain size is relatively large, steel plasticity first increases with grain refinement. However, when grain size is reduced below the critical grain size, further refinement causes rapid plasticity reduction. According to the model established in this work, the critical grain size at which X80 pipeline steel plasticity begins to decrease rapidly with grain refinement is approximately 2.5 mm. Compared with our previous work, the critical grain size predicted in this work shows better agreement with experimental data.

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Note: Figure translations are in progress. See original paper for figures.