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Modeling of the Size Effects on the Behavior of Metals in Microscale Deformation Processes

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For the accurate analysis and design of microforming process, proper modeling of material behavior at the micro/mesoscale is necessary by considering the size effects. Two size effects are known to exist in metallic materials. One is the "grain size" effect, and the other is the "feature/specimen size" effect. This study investigated the feature/specimen size effect and introduced a scaling model which combined both feature/specimen and grain size effects. Predicted size effects were compared with three separate experiments obtained from previous research: a simple compression with a round specimen, a simple tension with a round specimen, and a simple tension in sheet metal. The predicted results had a very good agreement with the experiments. Quantification of the miniaturization effect has been achieved by introducing two parameters, α and β, which can be determined by the scaling parameter n, to the Hall–Petch equation. The scaling model offers a simple way to model the size effect down to length scales of a couple of grains and to extend the use of continuum plasticity theories to micro/mesolength scales. [DOI: 10.1115/1.2714582]

Keywords: microforming, miniaturization, scaling effect, size effect

1 Introduction

A general trend towards highly integrated, compact products, and increasing applications in the area of microsystems demand further miniaturization of the required components. In 1990s, as the awareness and the need for microsystem technology grew, the manufacturing industry used microfabrication techniques such as lithography for silicon-based components. For metallic components, traditional turning and milling processes were scaled down to produce mesoscale parts [1–3]. From the viewpoint of metal forming, production of such miniature parts drew attention since forming is the most commonly used method of manufacturing near net shape parts, especially when mass production and high production rates are of concern [4]. Applied research in the areas of miniature scale bending [4], microextrusion [4–8], coining [9–11], and microdeep drawing [12] has expanded over the recent years. It was recognized, however, that the knowhow of traditional metal forming processes cannot be easily scaled down to microforming due to scaling effects.

In order to simulate the microforming process accurately, appropriate models for material behavior across a large range of size scales are necessary. As the material evolves through a sequence of manufacturing steps, so must the constitutive equations representing them. Nevertheless, lack of available material models and complications associated with linking different size scales limited the utilization of simulation tools [13]. There may be several approaches one could take to overcome this. One approach may be to start from the basic molecular dynamics. As pointed out by Horstemeyer [14], however, current computing power restricts the use of molecular dynamics technology to 10^{-6} m in the length scale and 10^{-8} s in the time scale, at most. On the other hand, continuum models are currently available down to millimeter and millisecond range. The inclusion of constitutive equations containing a physical size scale in the continuum models, the approach undertaken in this study, can extend its application to micrometer ranges [13].

As miniaturization occurs, scaling effects take place and the resulting consequences vary depending on the length scales. As the size of a polycrystal specimen approaches the size of a grain, many researchers have observed a decrease in the flow stress [4,5,15,16]. As the length scale of the part further decreases to a couple of micrometers, however, hardness and yield strength of metals increase because of the higher-order effects [17–19]. In these micrometer length scales, researchers attempted to explain the phenomena using the strain gradient plasticity theory [20,21]. The scope of this study is restricted to the specimen length scales down to the size of a couple of grains, typically around 100 μm at which the higher-order effects are negligible.

This size effect is thought to originate from two distinctly different sources, as shown in Fig. 1. The first is the "grain size" effect, which does not involve scaling of the feature or specimen size. This effect has been extensively studied by material scientists. The other is the "feature size" or "specimen size" effect, which actually involves geometrical scaling of the workpiece. Surprisingly, not much research has focused on the feature/specimen size effect and its interactions with the grain size effect at the length scale of a few hundred micrometers. Miyazaki et al. noted the decrease of the flow stress as the specimen size decreased and explained the trend by analyzing the "affected zone" of a deformed grain [22,23]. With a similar concept of surface grains being weaker than internal grains, Engel and co-workers developed a "surface layer model" [4,5,15,16,24,25]. The study conducted by Nakamachi et al., however, suggests that the weakening of the polycrystalline material for large grains is due to stress localization caused by reduced restriction from neighboring grains rather than weakening of the surface grains [26].

This study investigates the feature/specimen size effect and quantifies it by relating it to the fundamental properties of single and polycrystal deformation. After presenting the background in-

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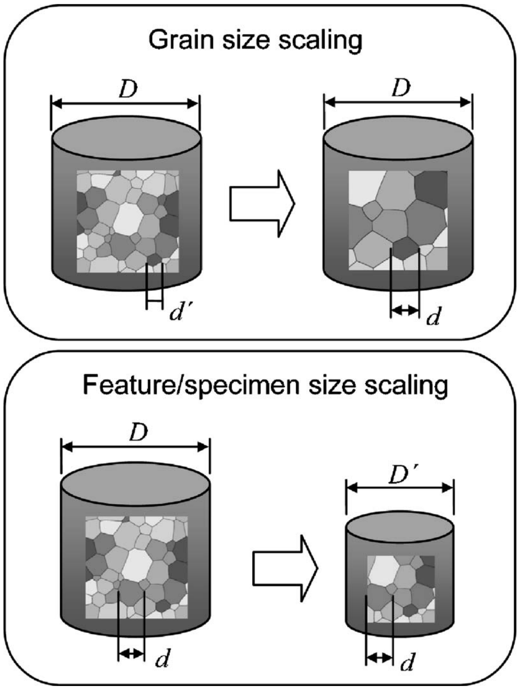


Fig. 1 Illustration of two types of scaling effects: the "grain size effect" and the "feature/specimen size effect"

formation in the next section, the formulation of the proposed scaling model that includes the two different size effects is presented. The model has been compared with experimental data retrieved from previous studies for validation. A summary and discussion of the results are then presented in the last section.

2 Background-Size Effects

As pointed out by Armstrong [27] in 1961, there are two types of size effects when considering the plastic flow of polycrystals. The first is the grain size effect, which has been investigated by numerous researchers. One of the most widely accepted empirical theories relating the yield stress to the grain size is the Hall–Petch equation [28,29], which was further extended by Armstrong to include the flow stress region [30]

$$\sigma(\epsilon) = \sigma_0(\epsilon) + \frac{k(\epsilon)}{\sqrt{d}} \tag{1}$$

$\sigma_0(\epsilon)$ and $k(\epsilon)$ are constants at a specific strain (ϵ), and d is the grain size. The first term, $\sigma_0(\epsilon)$, is known as the friction stress required to move individual dislocations in microyielded slip band pileups confined to isolated grains, whereas $k(\epsilon)$ in the second term measures the locally intensified stress needed to propagate general yielding across the polycrystal grain boundaries [31]. Therefore, the equation makes it possible to separately understand and analyze the contributions from the grain interior and boundary on the overall flow stress of a material [32].

Armstrong suggested that the values of $\sigma_0(\epsilon)$ obtained from Hall–Petch analysis could be related to the resolved shear stress τ_R, a single crystal property, as shown below [31]

$$\sigma_0(\epsilon) = M\tau_R(\epsilon) \tag{2}$$

where M is the orientation factor to account for slips on deformation systems. The orientation factor, M, is the average value of all the different orientations of the grains constituting the whole specimen. Thus, $\sigma_0(\epsilon)$ may be considered as the flow stress of a single crystal oriented for multislip [33]. The Taylor model, an upper-bound model that assumes the strains to be the same in all grains and equal to the macroscopic strain, requires at least five

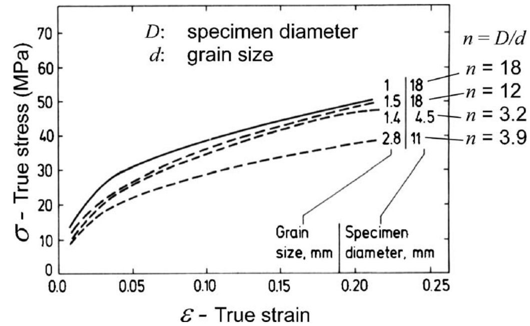


Fig. 2 Stress–strain curves of 99.999% aluminum for various *n* values [36]

active slip systems. The Sachs model, a lower-bound model, which assumes equal stress in all grains, requires only one active slip system [34]. For face-centered cubic (fcc) crystals, M is found to be 3.06 and 2.23 for the Taylor and Sachs model, respectively [35]. Combining Equations (1) and (2), we can express the polycrystal flow stress with the grain size, d, resolved shear stress, τ_R, and grain boundary resistance, k, in the following form

$$\sigma(\epsilon) = M\tau_R(\epsilon) + \frac{k(\epsilon)}{\sqrt{d}} \tag{3}$$

The first term in Eq. (3) relates the polycrystal flow stress to the single crystal flow property, and the second term adds the grain boundary resistance and grain size contribution to the flow stress.

The second effect that needs to be considered in miniaturization is the feature size or the specimen size effect and its interaction with the grain size. This feature/specimen size effect has received relatively less attention compared with the grain size effect until recently, since most deformation processes dealt with large part sizes, which could be considered as polycrystals. With an increasing trend toward miniaturization, the relationship between the grain size and the feature/specimen size needs to be considered and properly accounted for when modeling material behavior in the micro/mesoscales.

Hansen [36] reported that the strength of multicrystalline specimens, meaning specimens containing only a small number of grains across the cross section, decreases with a decreasing number of grains in the cross section, as shown in Fig. 2. As the grain number (n) or the number of grains across the cross section reduces to about four, the flow stresses also decrease accordingly. As the number of grains across the cross section further decreases to only a couple of grains, $n \sim 3.0$, decreasing the flow stress suddenly exhibits a large variation (i.e., for the case of $n=3.2$ in Fig. 2). When the grain number is smaller than $n < 3$, the local grain orientation becomes dominant and exerts a significant influence on the flow stress. Therefore, the flow stress, in this size range, will mostly depend upon the texture or the local orientation of the grains. Similarly, for sheet metals, Janssen investigated cases where the thickness of the specimen was below two to three grains and found distinctly different behavior of the sheet metal in these regions [37].

Armstrong described the condition whereby a specimen size effect allows earlier yielding of a material whose grain structure is intermediate between that of a single crystal and a true polycrystal in terms of inequality [31]

$$2\tau_R \leqslant \sigma \leqslant M\tau_R + \frac{k}{\sqrt{d}} \tag{4}$$

Figure 3 shows a number of flow stress measurements for reasonably pure aluminum at different grain sizes and also at different specimen sizes, as reported by Carreker and Hibbard [38], Fleischer and Hosford [39], and Hansen [36]. Carreker and Hibbard measured the highest strength for the least pure material at the

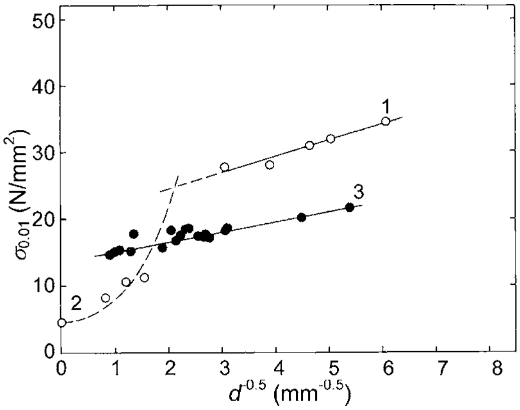


Fig. 3 Hall–Petch results for the polycrystalline aluminum [31]: (1) >99.987 Al [38]; (2) 99.992 Al et al. [39]; (3) 99.999 Al [36]

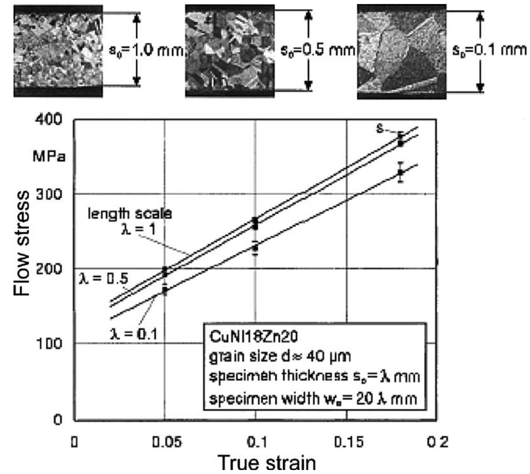


Fig. 5 Feature/specimen size effects in sheet metal [25]

smallest grain size. Fleischer and Hosford measured the lowest strength for material of intermediate purity but had only a few grains in the specimen cross section. Hence, Hansen argued that the specimen size effect was responsible for the Fleischer and Hosford data [39] falling below those data he reported after having employed very large specimen sizes with these large grain sizes (even for purer material) to ensure that polycrystalline deformation behavior was exhibited [36]. The results from Hansen show no sign of deviation from the Hall–Petch equation even with large grains.

Recently, feature/specimen size effect has received attention in the area of microforming for producing miniature parts (i.e., 100 μm–5 mm). Engel and his co-workers investigated scaling effects in CuZn alloys in the form of round specimens and sheet metals [4,5,15,16,24,25]. They employed the theory of similarity to study the size effect as part dimensions decreased. Figures 4 and 5 show the feature/specimen size effects in simple compression and sheet metal forming, respectively. In both figures, λ represents not only the geometric scaling factor, but also the scaling term that was used for the strain rate. In the size scales considered in this study where the part size is at least the size of a couple of grains, flow stresses decreased with miniaturization.

The fundamental physics underlying the size effect is still not fully understood. Different deformation mechanisms may be dominant at different size scales. For instance, the surface energy may be dominant on the nanometer scale [40], while geometrically necessary dislocations and strain gradients may be more active on the micrometer scale [21,41,42]. For the size scales considered in this study when part dimensions are several times the grain size, Engel and co-workers proposed the surface layer model to qualitatively describe the feature size effect [25]. In the surface layer model, a specimen is subdivided into a free surface and an internal portion. The model argued that the free surface did not represent a boundary comparable to a grain boundary, and thus the dislocation movement in surface grains was not restricted in the same way as in internal grains, yielding a less distinct hardening. Therefore, it was concluded that the flow stress of the surface portion is weaker than that of the internal portion of a material. Recent findings by Han et al., however, suggested that the free surface may exhibit either stronger or weaker resistance to plastic deformation, depending on the density of surface dislocation sources [42]. Also, mentioned in the work of Janssen is the possible influence of a boundary layer such as a native oxide layer may have on the dislocation motion in the surface grains [37]. Hence, the assumption that the surface layer is always weaker than the internal portion is questionable in certain circumstances.

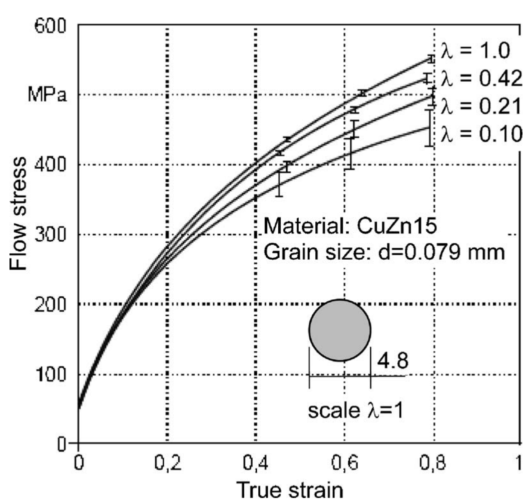
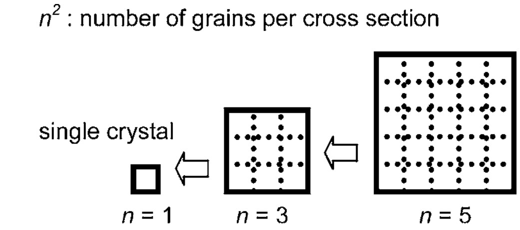


Fig. 4 Feature/specimen size effects in round specimens [4,5,15,16,24]

3 Formulation of the Scaling Equation

In this study, a different approach has been used to explain and quantitatively model the feature/specimen size effect. Equation (4), proposed by Armstrong, suggests that the flow stress of a polycrystalline material should decrease to the flow stress of a single crystal as the specimen size is decreased. In achieving this general hypothesis, the following detailed analysis and assumptions have been made in this study.

In Eq. (3), the second term is related to the contributions from the grain boundary to the total flow stress. For the case of a single crystal, however, there are no neighboring grains to resist the propagation of dislocations, and consequently there would be no effect induced by the grain boundary. The internal grain boundary length per area (GB_i/area) decreases as the size of the specimen is decreased, and eventually becomes 0 for a single crystal. This is explained in Fig. 6 for the ideal case of square-shaped grains and specimen cross section. As the number of grains (n) increases, the internal grain boundary per area (GB_i/area) increases from 0 to 2 for the square grains. Hence, for a given grain size, when the specimen size decreases from a polycrystal to a single crystal, the effects induced by the grain boundary will diminish. The assumption may be represented in the following form



n	1	3	5	7	10	20	∞
GB_i/Area	0	1.33	1.60	1.71	1.80	1.90	2

Fig. 6 Illustration of reduction of internal grain boundary length per area (GB_i/area) with miniaturization

$$\sigma(\epsilon) = M\tau_R(\epsilon) + \frac{k(\epsilon)}{\sqrt{d}}\beta \tag{5}$$

where $0 \leqslant \beta \leqslant 1$; and β will be 1 for polycrystal and will approach 0 as the specimen size is reduced to a single crystal.

From the theory of single crystal plasticity, the deformation should follow the Schmid law illustrated in Fig. 7

$$\tau_C = (\cos\phi\cos\lambda)\sigma = m\sigma \quad \left(0 < m \leqslant \tfrac{1}{2}\right) \tag{6}$$

where τ_C is the critical resolved shear stress; and m is the Schmid factor. In Eq. (5), however, β becomes 0 and the second term vanishes for a single crystal, leaving only the orientation factor and the resolved shear stress. Thus, the value of M should converge to that of $1/m$ when specimen size approaches that of a single crystal, implying that M will vary with specimen size scaling with a minimum possible value of 2.

Furthermore, a comparison between the magnitude of the flow stress $\sigma(\epsilon)$ and the Hall–Petch constant $\sigma_0(\epsilon)$ supports that M is dependent on the specimen size scaling. In Fig. 8, the magnitude of the Hall–Petch constant $\sigma_0(\epsilon)$ is similar to the polycrystal flow stress for $n=18$, which is much higher than specimens with only a few grains across the cross section ($n=3.9$). Since the second term in Eq. (5) is positive for the material, the value of M must decrease as the n value is decreased, in order to represent the flow stress at the small n values. In other words, the value of $\sigma_0(\epsilon)$ is

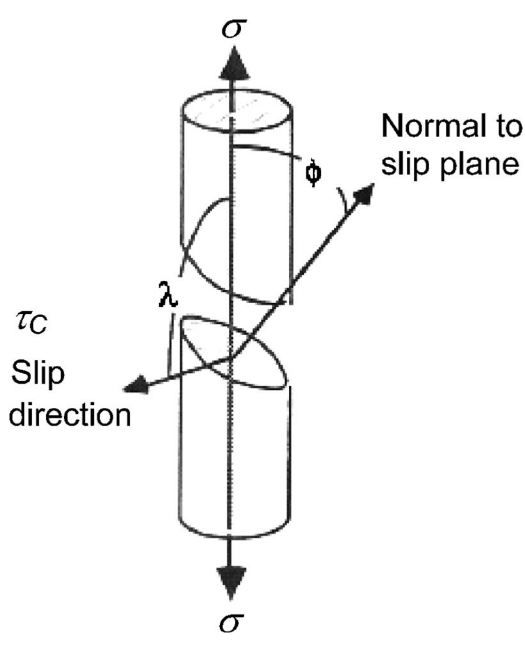


Fig. 7 Illustration of the Schmid law [45]

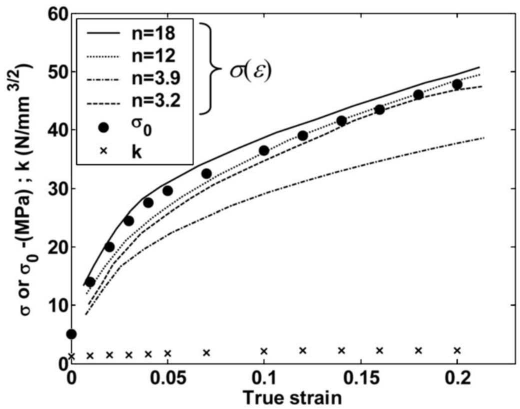


Fig. 8 Flow stress (σ) and Hall–Petch constants (σ_0 and k) as a function of strain for 99.999% Al [36]

not a constant but varies with respect to the ratio of the feature and grain size. Therefore, the following equation is proposed to describe the feature size scaling effect on M

$$\sigma_0(\epsilon) = M^\alpha \tau_R(\epsilon) \tag{7}$$

where ($M^\alpha \geqslant 2, \alpha \leqslant 1$); and α is 1 for a polycrystal.

Combining Eqs. (1), (5), and (7), a scaling equation including both the feature and grain size effects may be derived

$$\sigma(\epsilon) = M^\alpha \tau_R(\epsilon) + \frac{k(\epsilon)}{\sqrt{d}}\beta \tag{8}$$

where ($M^\alpha \geqslant 2, \alpha \leqslant 1, 0 \leqslant \beta \leqslant 1$); $\beta=0$ for a single crystal; and $\alpha=\beta=1$ for a polycrystal. It is also important to note the limitations and assumptions of the model. The model assumes that the grains are generally equiaxed, and thus the material behavior is assumed to be homogeneous. The model may be applied to parts that are fully polycrystal, down to parts that may contain only several grains. As the part size approaches the size of a single grain, the texture of the grain, rather than the averaged effect from the slip systems, dominates the behavior.

4 Results and Validation

Three sets of experimental data were used to evaluate and validate Eq. (8). Regarding the value of the orientation factor M, a study done by Lorentzen et al. [43] was employed. Figure 9 shows

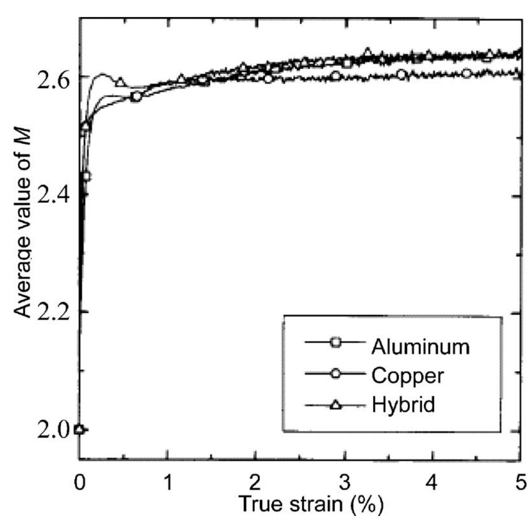


Fig. 9 The average value of orientation factor, *M*, for aluminum and copper [43]

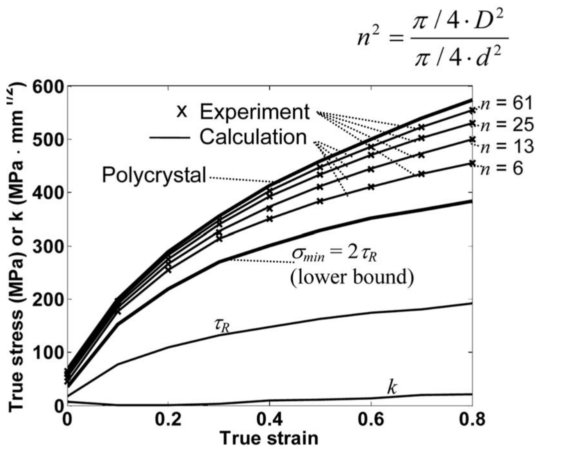


Fig. 10 Comparison of the experimental [4,5,15,16,24] and calculated results for the case of round specimens

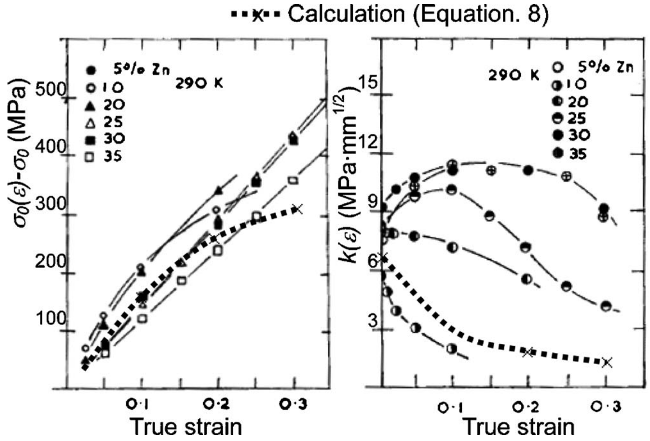


Fig. 11 Comparison of the Hall–Petch constants between the experiment [44] and the values obtained by calculation

the development of the average M value with increasing strain for aluminum and copper. After the initial low values in the elastic–plastic transition range, the M value finds stability at about 2.6. Thus, for all the calculations hereafter, the orientation factor M was assumed to be 2.6, about halfway between the values reported by the Sachs and Taylor models.

Equation (8) was first applied to experiments performed by Engel et al. shown in Fig. 4. They obtained flow stress curves from different specimen sizes through compression tests using round CuZn15 specimens that had uniform grain size of 0.079 mm for all the experiments. In Eq. (8), the true unknowns are α and β. Unfortunately, the values of $\tau_R(\epsilon)$ and $k(\epsilon)$ were unavailable for the given strain range, and thus they were also considered unknowns. To obtain the solution, an iterative approach was employed. After assigning an initial value to α and β, different sets of the flow stress curves were used to determine the $\tau_R(\epsilon)$ and $k(\epsilon)$ curves. An optimum solution of α and β will yield a minimum difference among the different sets of $\tau_R(\epsilon)$ and $k(\epsilon)$ curves. Hence, best-fit values of α and β may be determined through iterative procedures utilizing the experimental data shown in Fig. 4. (The calculated values for α and β are plotted in Fig. 14.)

Results predicted by simulation are shown in Fig. 10, where (×) represents the original experimental data. Calculated (—) results for each case of "n" match very well the experimental results. Predicted values for $\tau_R(\epsilon)$ and $k(\epsilon)$ were also compared with the experiments performed by Meakin and Petch for α brass containing Zn at levels of 5–35% [44]. As shown in Fig. 11, the two Hall–Petch constants agree with the experimental data for the available strain range up to 0.3. Experimentally measured k values after strain of 0.3 were unavailable, and thus a full comparison throughout the whole strain range was not possible. Although a strong variation of k was observed at higher strains, the calculated k values from different stress values did not deviate from one another, which confirms the accuracy of obtained values. According to the Schmid law, the minimum value of $\sigma_{\min}(\epsilon)$ is $2\tau_R(\epsilon)$. This is plotted in Fig. 10 and may be considered as the lower boundary for the material. It does not necessarily mean that the flow stress will converge to this curve when $n=1$, since the local grain orientation will determine the material behavior at this size. The polycrystal flow curve when $\alpha=\beta=1$ is also plotted for comparison.

A comparison between the model proposed in this study and the "surface layer model" of Engel [24] is presented as shown in Fig. 12. Overall, both models exhibit a similar trend in predicting the flow stress. As speculated by Engel [24], the flow stress of the inner portion of the specimen resembles the polycrystal behavior. According to Engel's model, however, the flow stress of the surface layer of the specimen is lower than that of the minimum single crystal flow stress calculated by our model.

The second set of experiments selected for validation was from Hansen [36] for cylindrical specimens of pure aluminum in tensile as shown in Fig. 2. For the case of Hansen, the Hall–Petch constants were given as shown Fig. 8. Thus, only α and β were considered unknowns in Eq. (8) when predicting the flow stress curves for various n values. The results are shown in Fig. 13. Except for the case of $n=3.2$, all other curves match very well the experimental values shown in Fig. 2. Hansen speculated that the higher flow curve obtained for $n=3.2$ was from the effect of the different crystal orientation. The inequality in Eq. (4) may be expressed in the following form to be more precise

$$\begin{array}{ccc} \text{(Polycrystal)} & & \text{(Single crystal)} \\ \sigma = M\tau_R + \dfrac{k}{\sqrt{d}} & \rightarrow & \sigma = \dfrac{\tau_R}{m} \end{array} \tag{9}$$

where

$$\left(\frac{1}{m} \geqslant 2\right)$$

As polycrystal material approaches the size of a single crystal, the flow behavior would resemble that of a single crystal, which is strongly affected by the crystal orientation, sometimes even higher than that of the polycrystal. Consequently, it is expected that the crystal orientation will have a strong influence when the n value is close to 1.

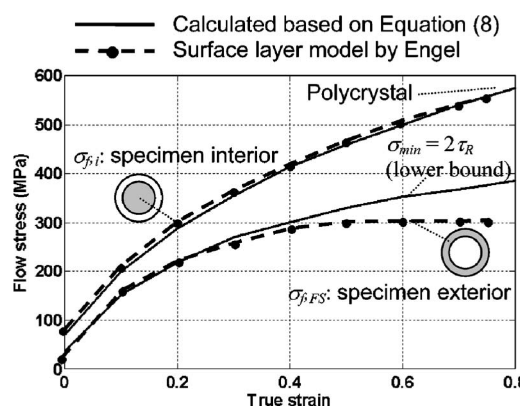


Fig. 12 Comparison of flow stresses calculated by Eq. (8) and "surface layer model" by Engel [24]

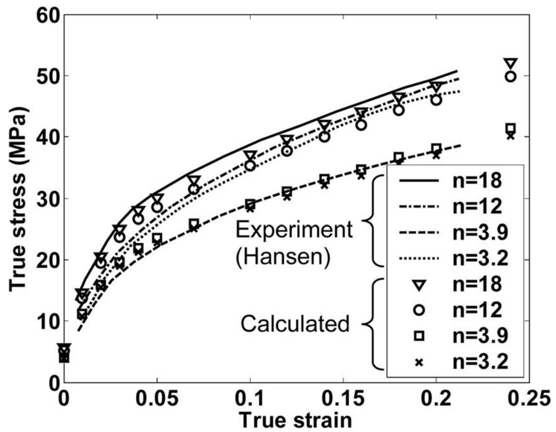


Fig. 13 Calculated results using Eq. (8) based on the experiment by Hansen [36]

The parameter values of α and β for the previous two simulations are summarized in Fig. 14. As expected, both parameters approach the asymptotic value of 1 for the polycrystal as n is increased. As n decreases to 1, β decreases to 0 and α reaches the value of 0.73 which yields the minimum value for $1/m$ $(=M^{\alpha} = 2.6^{0.73} = 2.0)$ in Eq. (9). Thus, the values obtained from the simulation support the original assumptions for α and β. As shown in Fig. 14, parameter α had a more dramatic drop than β as n decreased. The limit of $n=15$ was suggested by Hansen as when a specimen may start to show feature size effect [36], and the value corresponds to where a significant drop in α and β is observed.

Experimental data for tensile testing of sheet metal [25] were also used to evaluate the scaling equation. The experimental data and conditions are shown in Fig. 5. The experimental data were obtained for thicknesses of 1.0 ($\lambda=1$), 0.5 ($\lambda=0.5$), and 0.1 mm ($\lambda=0.1$) for the grain size of 0.040 mm. Since the $\tau_R(\epsilon)$ and $k(\epsilon)$ values were unknown, experimental data for $\lambda=0.1$ and $\lambda=1$ were used to calculate their values. Parameters α and β were obtained from Fig. 14, and n was calculated based on the cross section of the sheet metal. As shown in Fig. 15, the predicted flow stress for the case of $\lambda=0.5$ agreed very well with the experimental data.

All three sets of predicted results reproduced the experimental data very well, validating the scaling model in the form given by Eq. (8). From the analysis, it is speculated that the parameters α and β are independent of the material but are governed by the scaling parameter n, although more evidence and proof are required to expand the application of the model to all polycrystal materials.

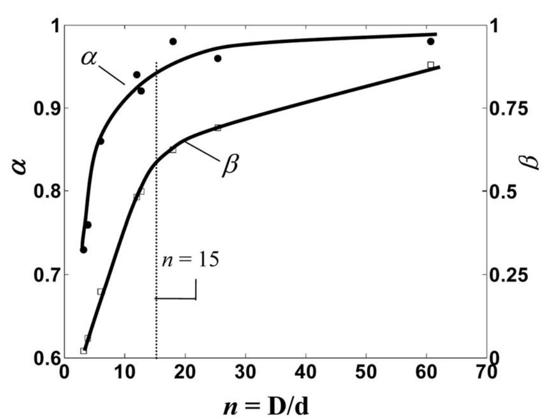


Fig. 14 Parameters α and β, and their dependence on $n = D/d$ (D=feature size, d=grain size)

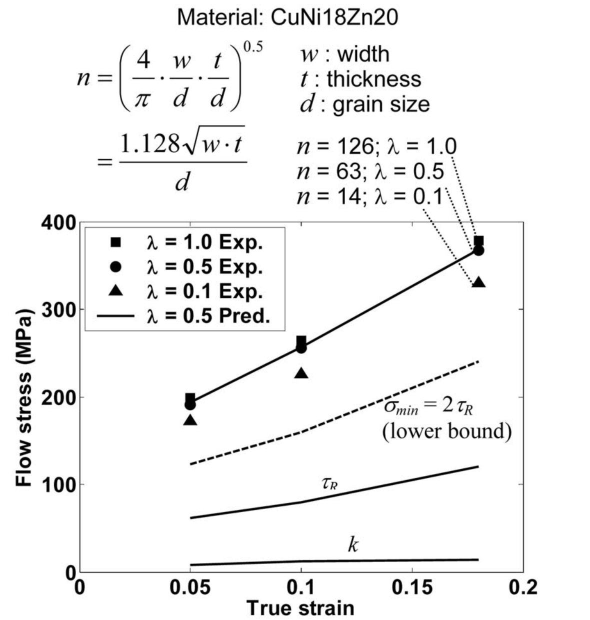


Fig. 15 Flow stress predicted and compared for $\lambda=0.5$ based on experimentally obtained values at $\lambda=0.1$ and $\lambda=1.0$ for sheet metal

5 Conclusions

In this study, we proposed a model that can quantify the relationship between the "grain size" and the "feature/specimen size" effect based on the phenomenological experimental results. A scaling model was derived based on the hypothesis that a polycrystal material should recover the fundamental stress–strain relationship of a single crystal as the specimen size is decreased to the size of a single grain. By introducing two parameters, α and β, to the Hall–Petch equation, the scaling equation was proposed to describe the interactions between the "feature/specimen size" and the "grain size" effect as in Eq. (8).

The scaling equation was used to reproduce three different cases of experimental results reported in previous studies: (1) a simple compression with a round specimen [4,5,15,16,24]; (2) a simple tension with round specimen [36]; and (3) a simple tension in sheet metal [25]. In all three cases, the stress–strain relationship predicted by the scaling equation had a good agreement with the experimental results. As the miniaturization of the specimen occurred, the first term in Eq. (8), $M^{\alpha}\tau_R$, approached the minimum value predicted by the Schmid law, $2\tau_R$, and the second term, $(k/d^{0.5})\beta$, which is related to the resistance from the grain boundary, disappeared as the specimen size decreased to that of a single crystal.

This study suggests and confirms that the material flow stress depends not only on the grain size but also on the interactions with the specimen/feature size. The Hall–Petch relationship describes the dependence of the flow stress on the grain size in polycrystal materials. As miniaturization occurs, the flow stress converges to that of a single crystal. The flow stress continuously decreases until the part size is that of a couple of grains at which point the local crystal orientation starts to dominate the material behavior. Quantification of the miniaturization effect has been achieved through n value which is defined as the ratio of specimen/feature size to the grain size. n becomes 1 for a single crystal and ∞ for polycrystals. The values of α and β in Eq. (8) and their dependence on n value, quantify the flow stress dependence on miniaturization.

The scaling model proposed in this study provides the means to extend the use of continuum plasticity-based finite element simulation tools to micro/mesolength scales cost effectively. The findings and the proposed model, however, need to be further validated with experiments involving various microforming processes.

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