Virtual design of formability for Zircaloy-4 sheet through texture control

H Liu¹,², S Deng¹, S Chen¹, H Song¹, S Zhang¹*

¹ Shi-changxu Innovation Center for Advanced Materials, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China
² School of Materials Science and Engineering, University of Science and Technology of China, Shenyang 110016, China

* Corresponding author: shzhang@imr.ac.cn

Abstract. Zircaloy-4 (Zr-4) sheet is commonly used in fuel assembly structural parts as spacer grids which are subjected to high temperature and stresses, corrosive and radiation environment. The knowledge regarding the properties and the formability with respect to initial texture of Zr-4 sheet is not enough. In this paper, finite element method was used to simulate the forming process of Zr-4 sheet, and effect of different initial hardening exponent (n value) on the formability of sheet is studied. The results show formability of sheet reveals better with larger n value. However, the hardening exponent (n value) is closely related to the features of initial texture of sheet. Thus, the well-established polycrystal plasticity method, visco plastic self-consistent (VPSC) model, was used to predict the effect of different initial textures on the hardening exponent of Zr-4 sheet, and plastic deformation mechanism of different initial textures in stamping process was analyzed. The results show that a larger the hardening exponent is obtained under a smaller normal Kearm factor (Fn) of the initial texture, and the activation of prismatic slip decreases with increasing the Fn.

1. Introduction
Zirconium alloys featured with excellent corrosion resistance and mechanical properties are widely using in nuclear power and aerospace fields [1-3]. The strip components of zirconium alloy in the nuclear power industry requires to be produced with suitable stamping process to ensure their successive fabrication with good quality [4, 5]. Therefore, research on the formability of zirconium alloy sheet is very necessary. Generally, there are many factors which affected the formability of zirconium alloy sheet. Among them, the initial texture of Zr-4 sheets is one of the important factors. Zhang [6] et al.
investigated the stamping formability of Mg–3Al–1Zn (AZ31) alloy was greatly enhanced through weakening (0001) basal texture by repeated unidirectional bending. Swadesh Kumar Singh [7] et al. studied the formability of Zircaloy-4 sheets produced through pilgering route, and the prepared direction of specimen has negligible influence on Forming Limit Diagram (FLD) in tension–tension region and marginally influence in tension–compression region. Murty and Charit [8] reported that the developed crystallographic texture significantly affects subsequent formability and in-service performance with HCP alloy during deformation.

In order to study the influence of different initial texture of zirconium alloy on the formability during stamping process. Stamping process of Zr-4 sheets was investigated with finite element method in this paper. The effect of different hardening exponent on formability was studied, and then the relationship between hardening exponent and initial texture was built by visco-plastic self-consistent (VPSC) model. The deformation mechanism of effect of different initial textures on formability was clarified during stamping process to find the optimal texture for stamping process of zirconium alloy sheet.

2. Experimental method and Material

2.1 Material model

The material used in this study was Zircaloy-4 sheet with an initial thickness of 0.5 mm. Its Young’s modulus and Poisson’s ratio were assumed to be 100 GPa and 0.42. The specimens were machined using wire-electrode cutting along rolling direction (RD), 45 to the rolling direction (45RD) and transverse direction (TD), as shown Figure 1 (a). The dimensions of tensile specimens are 15 mm in width and a gauge length of 50 mm. Anisotropic tests were performed with a Zwick-Z050 tensile machine at a low strain rate of 0.001 s\(^{-1}\). During the tests, two extensometers along axial and transverse directions were used to estimate the r value which defined by the ratio between transverse strain and thick strain at an elongation about 10% –15%. The yield model provided with Barlat-89 [9] are used to obtain anisotropic properties for Zr-4 sheets. The experimental mechanical properties given in Table 1 are used as input data in the identification procedure to obtain the coefficients of yield criterion. The hardening exponent n value is evaluated with typical Holloman hardening law defined by equation (1).

\[
\sigma = K\varepsilon^n
\]  

where \(\sigma\) is true stress , \(\varepsilon\) is true strain and K is hardening coefficient.

The flow stress curve of Zr-4 sheet which shows in Figure 1 (b) is another important parameter in finite element simulation. With the increasing angles from rolling direction, the yield stress increases. Both the tensile stress and n value decrease from 0° to 45°, while they keep almost the same for 45° and 90°. The r value firstly increases then decreases from 0° to 90°. The anisotropy is obvious which will influence the formability of Zr-4 sheet during stamping process.
Figure 1. (a) Schematic illustration of specimens in Zr-4 sheet (b) True stress vs. strain of Zr-4 sheet for various directions.

Table 1. Mechanical and anisotropic properties of Zircaloy-4.

| Loading direction (°) | Yield stress (MPa) | Tensile stress (MPa) | r  | n  |
|-----------------------|--------------------|----------------------|----|----|
| 0                     | 401.7              | 487.7                | 4.744 | 0.13 |
| 45                    | 414.6              | 462.7                | 6.514 | 0.11 |
| 90                    | 432.4              | 466.1                | 6.279 | 0.10 |

2.2 The finite element (FE) model
The stamping process is simulated by finite element method using Dynaform5.9.4 software. Figure 2 shows the FE model including punch, binder, blank and die. The blank mesh type used in the model is Belytschko-Tsay shell element, while tool parts are set as rigid body. Mesh size of blank is 0.05 mm. The total number of blank mesh is 19685. The contact type is CONTACT_FORMING_ONE_WAY_SURFACE_TO_SURFACE_ID. The coulomb friction coefficient was assumed to be \( \mu = 0.125 \) for both the upper and bottom surface of blank. The material model is 36*MAT_3-PARAMETER_BARLAT. Barlat89 yield criterion and Swift hardening model was selected during forming. The yield criterion is suitable for materials with internal anisotropy under plane stress conditions. The initial blank size is 17 mm x 8.8 mm. The punch velocity is 5000 mm/s to accelerate the simulation process, binder velocity is 100 mm/s and binder force is 2000 N.

Figure 2. Finite element model of stamping process of Zr-4 sheet.
3. Effect of hardening exponent on formability in stamping

The formability of the material is closely related to the material characteristics, especially the hardening exponent. In order to study the influence of different hardening exponents on the formability, stress and wall thickness of sheet at six typical positions were studied with the results of finite element simulation.

Figure 3 shows the distribution of stress and wall thickness at six typical positions. In Figure 3(a), the stress is lowest at the bottom position and peak at the angle rounded of die where the deformation is intense and the stress is concentrated, while the distribution of stress is roughly same with the n value from 0.12 to 0.2. The equivalent stress of the cross section decreases gradually with increasing n value, the formability of sheet is better during stamping process. In Figure 3 (b), the distribution of wall thickness is the peak at edge position, and wall thickness at straight-sided occurs a growth. With increasing n values, the distribution of wall thickness appears to be more uniform, which improves the formability of Zr-4 sheet in the stamping process and reduces the risk of fracture.

![Figure 3. Distribution at six typical positions under different hardening exponents (n value) (a) Stress (b) Thickness.](image)

Based on the above finite element simulation results, it can be concluded that when n value is larger, equivalent stress of the cross section decreases gradually and the distribution of wall thickness exhibits more uniform, and the improvement of formability will occur in stamping process of Zr-4 sheet.

4. Prediction of different initial textures on hardening index based on VPSC model

Forming limit of sheet is closely related to the hardening exponent. As mentioned above, the increasing hardening exponent lead to improvement the formability of Zr-4 sheet. The value of hardening exponent is largely attributed to the initial texture for Zr-4 sheet. To obtain the relationship between the initial texture and hardening exponent, VPSC model is built to predict mechanical behavior under tension along rolling direction. Detailed theory on VPSC model can be found in Refs [10, 11]. The Kearns factor is employed to quantitively describe the grain orientations with basal poles lying along a particular sample axes, which can be calculated via equation (2). It is specified that Fr, Ft and Fn represent Kearns factor with the rolling direction, transverse direction and normal direction, relatively.

\[
F = \frac{\int_0^\pi I_\varphi \sin \varphi \cos^2 \varphi \, d\varphi}{\int_0^\pi I_\varphi \sin \varphi \, d\varphi}
\] (2)
where $I_\phi$ is the average intensity at a tilt angle $\phi$.

Typical bimodal texture with five different $F_n$ values were used to illustrate the effect of initial texture on hardening exponent. Figure 4 shows the normal Kearn factor ranging from 0.605 to 0.721 for (0001) pole figure as initial texture used in VPSC. After calculation, the predicted stress-strain curves were obtained as Figure 5. The results showed that both yield stress and stress-strain curves increased with increasing normal Kearn factors. Normally orientated crystals with higher $F_n$ are detrimental to the hardening ability with lower $n$ value.

![Figure 4](image)

**Figure 4.** (0001) pole figures and Kearn factors of different initial textures.

![Figure 5](image)

**Figure 5.** Predicted strain-stress curves of Zr-4 sheet under different initial textures.

| Initial texture | $F_r=0.045$ | $F_r=0.059$ | $F_r=0.074$ | $F_r=0.076$ | $F_r=0.077$ |
|-----------------|-------------|-------------|-------------|-------------|-------------|
| $F_t=0.349$     | $F_t=0.261$ | $F_t=0.235$ | $F_t=0.222$ | $F_t=0.202$ |
| $F_n=0.605$     | $F_n=0.680$ | $F_n=0.691$ | $F_n=0.702$ | $F_n=0.721$ |

**Table 2.** Effect of Kearn factor on hardening exponent ($n$ value).

The variation of mechanical property could be attributed to the relative contribution of deformation mechanisms with straining. Figure 6 shows the differences in prismatic slip activity under tension along
RD under various initial textures. It discloses that with the grain orientation being more close to normal direction (i.e, (0001) direction), the prismatic slip activation become larger. As the easiest activated mechanism among four different deformation mechanisms in Zirconium alloys [12], the larger amount of its activation of prismatic slip will lead to a relative lower yield stress and stress-strain curve. That is, the yield stress and ultimate tensile stress become higher with more activation of harder modes, such as pyramidal <c+a> slip and basal <a> slip. As can be seen, the prismatic slip dominates the whole tensile deformation under different initial texture. Additionally, prismatic slip exhibits better self-hardening ability than other non-prismatic slip modes. Therefore, the one with smaller Fn has the highest activity of prismatic slip, which in turn contributes a good hardening ability and a higher hardening exponent n value. Thus, a good formability of Zr-4 sheet can be expected under the smaller Fn.

![Figure 6. Effect of Kearn factor on the relative activity of prismatic slip.](image)

5. Conclusion

In this work, the influence of different hardening exponents on the formability of Zr-4 alloy sheet was studied by the finite element method. The relationship between the initial texture and hardening exponents was studied by the VPSC model, clarifying the deformation mechanism. The relationship between texture feature and formability was indirectly established, and main results can be drawn as follows:

1. A larger n value is obtained with reducing normal Kearn factors (Fn), and resultantly a better formability of Zr-4 alloy sheet is obtained during stamping.
2. Stress-strain curves and hardening exponent rose with increasing normal Kearn factors of initial texture.
3. The activation of prismatic slip decreases gradually during the deformation process. With the increase of Fn, the activation of prismatic slip decreases gradually.

References

[1] Cox B 2005. Some thoughts on the mechanisms of in-reactor corrosion of zirconium alloys. *J. Nucl. Mater* 336 331-368
[2] Krishna K V M, Sahoo S K, Samajdar I, Neogy S, Tewari R, Srivastava D, Dey G K, Das G H,
[3] Long F, Xu F and Daymond M R 2013 *Metall. Mater. Trans. A* **44** 4183-93
[4] Takuda H and Hatta N 1998 *Mater. Sci. Eng. A* **242** 15-21
[5] Takuda H, Kikuchi S and Hatta N 1998 *J. Mater. Process. Technol* **84** 117-121
[6] Huang X, Suzuki K, Chino Y and Mabuchi M 2013 *Mater. Sci. Eng. A* **565** 359-372
[7] Singh, S K, Limbadri, K, Singh A K, Ram A M, Ravindran M, Krishna M, Reddy M C, Suresh K, Prasad K S and Panda S K 2019 *J. Mater. Res. Technol* **8** 2120-29
[8] Murty L K and Charit I 2006 *Prog. Nucl. Energ* **48** 325-359
[9] Barlat F and Lian K 1989 *Int. J. Plast* **5** 51-66
[10] Lebensohn R A and Tomé C N 1993 *Acta Metall. Mater* **41** 2611-24
[11] Tomé C N, Lebensohn R A and Kocks U F 1991 *Acta Metall. Mater* **39** 2667-80
[12] Deng S Y, Song H W, Liu H and Zhang S H 2021 *Int. J. Solids Struct* **213** 63-76