Texture Transformations and Its Role on the Yield Strength of ($\alpha+\beta$) Heat Treated Zircaloy–4

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($\alpha+\beta$) 열처리된 지르칼로이-4에서 집합조직의 변화와 그 조직이 항복 강도에 미치는 영향

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(1991. 9. 2 접수)

Abstract

The texture changes and their effect on the 0.2% yield strength of Zircaloy–4 sheet were examined after quenched from the ($\alpha+\beta$) phase temperature. When the prior ($\alpha+\beta$) grain size was slightly larger than that of the α–annealed, the observed texture was similar to the α–annealed texture having an ideal orientation of the (0001) basal pole at 30° away from the normal direction toward the transverse direction. When the prior ($\alpha+\beta$) grain size was twice as large as that of the α–annealed, the location of maximum basal pole intensity was distributed between the transverse and the rolling direction making an angle 15° from the normal direction, and the observed texture became isotropic. It was found that the Kearns texture parameter, f_r in the rolling direction increased steadily, and f_t in the transverse direction increased slightly, while f_n in the the normal direction decreased with increasing heat treatment time. With a small increase in f_r, the 0.2% yield strength increased drastically. The influence of texture was analyzed by deriving the Schmid orientation factors and the resolved shear stresses for the deformation systems. It was found that the large increase in the 0.2% yield strength was attributed mainly to the microstructural changes and partly to the texture changes by the ($\alpha+\beta$) heat treatment.

요 약

($\alpha+\beta$) 영역에서 급냉된 지르칼로이-4 판재 시편에서 집합조직의 변화와 그 조직이 0.2% 항복강도에 미치는 영향에 대하여 조사하였다. ($\alpha+\beta$) 입자의 크기가 α 영역에서 소둔된 시편의 입자 크기보다 약간 클 경우 관찰되는 집합조직은 α-소둔된 시편의 것((0001) 기저폴은 수직 방향에서 횡 방향으로 30° 기울어져 분포)과 비슷하였다. ($\alpha+\beta$) 입자 크기가 α-소둔된 시편의 입자 크기보다 2배 정도로 커지면서 기저폴의 최대치는 수직 방향에서 횡 방향 및 압연 방향으로 약 15° 기울어져 분포하여 집합조직은 등방성을 가졌다. 열처리 시간이 길어질 수록 Kearns의 집합조직 변수 f는 압연 방향에서 증가하였고 횡 방향에서는 약간 커졌으며 수직 방향에서는 계속 감소하였다. 압연 방향의 f가 조금 증가함에 따라 0.2% 항복강도는 크게 증

가하였다. 변형 기구에 따른 Schmid인자와 분해전단응력을 구하여 집합조직이 항복강도에 미치는 영향을 조사하였다. 급격한 항복강도의 증가는 주로 미세조직의 변화에 기인하였으며 집합조직이 미치는 영향은 상대적으로 작았다.

I. Introduction

Due to an anisotropic crystalline property, a preferred orientation, or a texture, is well developed in the zirconium and its alloys [1-3]. The texture of an as-received Zircaloy-4 sheet showed an ideal orientation, in which the (0002) basal poles were distributed in the normal-transverse plane of the sheet with the maximum tilt angle of the basal poles at 30° from the normal direction [4-6]. The quantitative description of textures in Zircaloys can be made possible by the introduction of Kearns [7] texture number, f-parameter. The orientation parameter, f, is the effective fraction of cells aligned with their [0001] axis parallel to the reference direction.

$$f = \int_0^{\pi/2} I(\phi)\sin\phi\,\cos^2\phi\,d\phi \qquad (1)$$

Several authors [3-6] have studied the development of textures by deformation and annealing of Zircaloys. The deformation texture observed in the α phase Zircaloy sheets was in the ideal orientation, where the $<10\bar{1}0>$ direction was parallel to the rolling direction [4-6]. When these materials were heated in the α phase region above the recrystallization temperature [8-9], the α-annealing texture was developed. Above this temperature, the α phase grains recrystallized and rotated 30 about the c-axis of the hcp(α) structure. Although, if recrystallization occurred, the orientation of c-axis was not changed. But, the $<11\bar{2}0>$ direction became parallel to the rolling direction [4, 5].

When the zirconium alloys were heated into the β(bcc) phase, the orientation changes would occur. Above 1273K, the α phase grains rapidly

transformed to β by the Burgers [10] relationship. As the grain growth of β phase grains was fast, the texture in the β phase would differ from the original α phase texture. When the alloys were cooled to room temperature, the different texture of the β transformed Zircaloy was produced. Glen and Pugh [11] predicted the theoretical textures after an $\alpha \to \beta \to \alpha$ transformation of zirconium crystals. The results showed that the theoretical textures appeared to be randomized due to many alternative orientations occurring by hcp→bcc→hcp transformation. Jung and Kim [12] also showed that the texture became randomized after the β heat treatment.

Ballinger and Pelloux [13] showed that in the cold-worked and stress-relieved Zircaloy-2 the uniaxial flow stresses were a function of the Kearns texture number, f. Jung and Kim [12] also derived a linear relationship between the 0.2% yield strength and the f-parameter in the axial direction from the deformation of the β transformed Zircaloy-4 cladding. Nakatsuka and Nagai [14] proposed a model which described the effect of crystallographic texture and stress state on the plastic deformation of Zircaloy cladding. The model predicted the operation of $\{10\bar{1}0\}$ $<1\bar{2}10>$ prism slip for axial tension. However, relatively little work has been reported on the texture changes and the corresponding effects on the mechanical properties by the $(\alpha + \beta)$ heat treatment. The $(\alpha + \beta)$ heat treatment would include the partial formation and growth of β(bcc) phase grains. The role of β phase grains on the texture development during the $(\alpha + \beta)$ treatment is still largely unknown.

The objective of the present study is to investigate the texture transformation by the $(\alpha + \beta)$ heat treatment and the corresponding effects on

the 0.2% yield strength. The texture measurement was done by X–ray diffraction, and the ensuing texture paraemeter, f–parameter, was calculated. The orientation dependent yield strength was found in the single crystal analogue by deriving Schmid[15] orientation factors and the resolved shear stresses for the prism slip and tensile twin.

2. Experimental procedure

The as–received Zircaloy–4 sheet was annealed at 873K for 2 hours in a vacuum furnace. Then, the $(\alpha + \beta)$ heat treatment was made at 1163K and at 1223K for 5, 10, 20, and 30min in the evacuated silica tubes and subsequently water quenched by breaking the tubes in water. The transformation product of the $\beta \rightarrow \alpha$ reaction will be designated as "transformed β" phase or α' in brief [16].

Sheet tensile specimens with a gage length of 35mm, a width of 6mm and a thickness of 0.8mm were prepared, and the loading axis of these specimens was parallel to the rolling direction of the as–received sheet. The tensile test of the $(\alpha + \beta)$ heat treated specimens was conducted at a strain rate of $9.5 \times 10^{-4} s^{-1}$ at a room temperature.

The crystallographic textures of the heat–treated specimens were measured by obtaining the direct pole figures and the inverse pole figures from the X–ray diffraction [17–19]. Samples for the pole figure analysis were chemically thinned to a thickness smaller than 95μm. The direct pole figure measurement was done by using combined Schulz transmission and Schulz reflection techniques where MoK$_\alpha$ was used for the X–ray source.

In the inveres pole figure measurement, composite specimens were prepared for each heat treated sample. Each specimen was mounted in a X–ray diffractometer and scanned for 2θ values of the Bragg's angle from 30° to 130° using CuK$_\alpha$ source. The area under (hk.1) reflection peak was used to calculate a texture coefficient value from

the equation [18]

$$T.C.(hk.1) = \frac{I(hk.1)/I_0(hk.1)}{\frac{1}{n}\sum_n I(hk.1)/I_0(hk.1)} \qquad (2)$$

where I(hk.1) is the measured integrated intensity of a given (hk.1) reflection produced by the textured specimen, I_0 (hk.1) is the intensity of the same (hk.1) reflection produced by a powder sample of random orientation, and n is the total number of reflections measured. A texture coefficient of unity denotes random orientation and the T.C. values of a plane is proportional to the number of grains with that plane parallel to the surface examined. The f–parameters were calculated from the T.C. values [7].

3. Results

3.1 Texture transformation

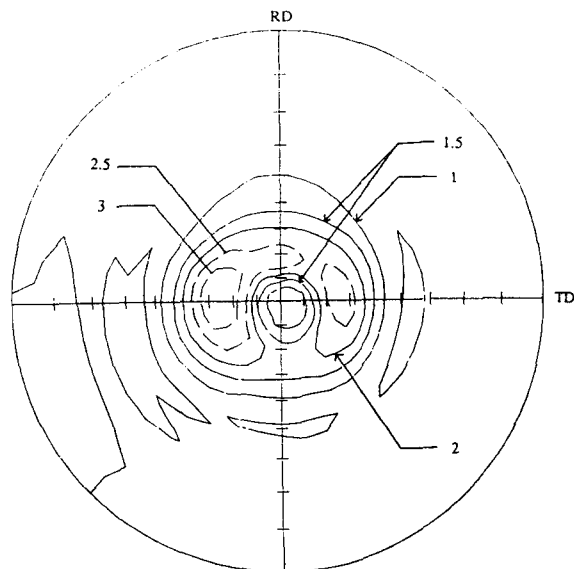Fig. 1 is the (0002) basal pole figure of the α

Fig. 1. (0002) Basal Pole Figure of Zircaloy–4 Sheet Heat Treated at 873 K for 2 hr.

–annealed Zircaloy–4 sheet. The idealized orientation of the (0001) basal pole is at 30° away from the normal direction toward the transverse direction. When the α–annealed specimen was heated for 5min at 1163K and at 1223K, respectively, the observed textures were similar to the α–annealed texture as shown in fig. 2(a) and fig. 3(a)

However, the location of maximum basal pole intensity was distributed between the transverse and rolling direction making an angle 15° from the normal direction when the samples were heat treated for heated for 30min at 1163K and at 1223K, respectively, as shown in fig. 2(b) and fig.
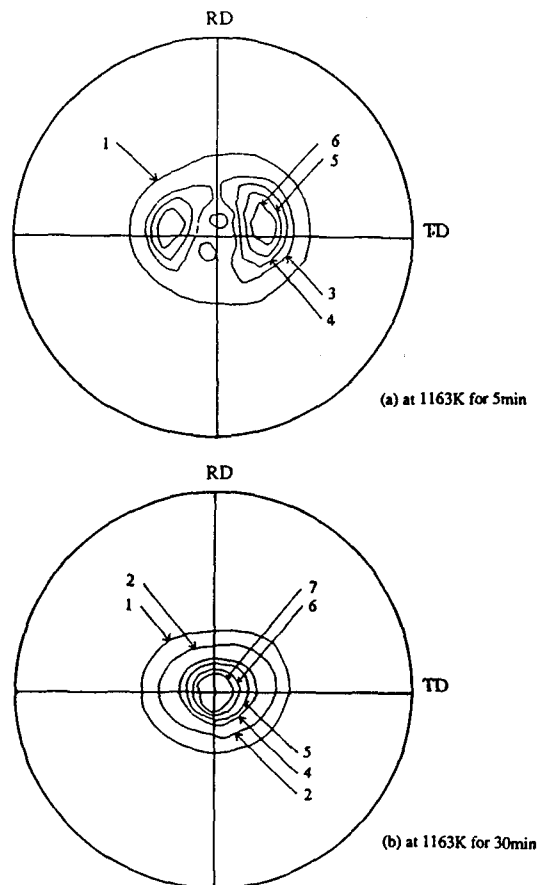

Fig. 2. (0002) Basal Pole Figure of Zircaloy–4 Sheet Heat Treated at 1163 K (a) for 5min, and (b) for 30min.
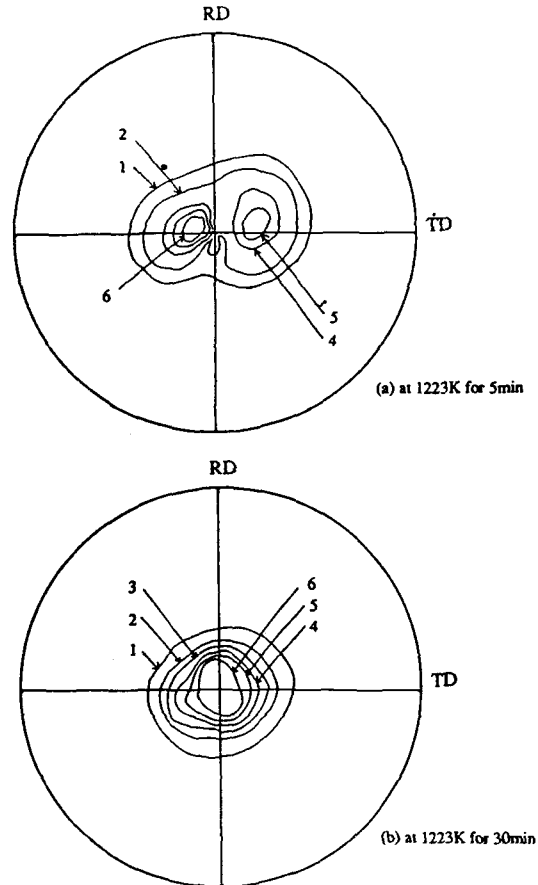

Fig. 3. (0002) Basal Pole Figure of Zircaloy–4 Sheet Heat Treated at 1223 K (a) for 6min, and (b) for 30min.

3(b).

These texture changes were quantitatively represented in the plot of Kearns texture number, f, from the results of the inverse pole figure measurements. In fig. 4, it is seen that the texture parameter, f_r in the rolling direction increases steadily, and f_t in the transverse direction increased only a little, while f_n in the normal direction decreases with increasing heat treatment time. It also exhibited that the (0001) basal poles became reoriented toward the rolling and transverse directions. The observed texture became more isotropic as the heat treating time increased.
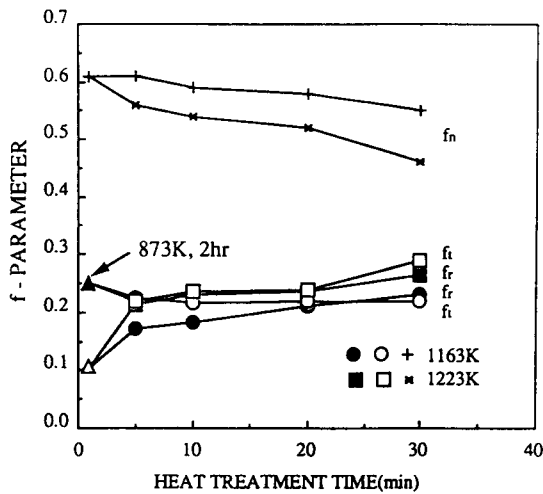
Fig. 4. Variation of f-Parameters with Heat Treatment Time.

3.2 The 0.2% yield strength

The variation of the 0.2% yield strength with f_r is shown in fig. 5. It is seen that the 0.2% yield strength increases with increasing f_r at 1163K and at 1223K treatments. The small increase in f_r resulted in the large increase in the 0.2% yield strength of the $(\alpha + \beta)$ heat treated samples. The two curves in fig. 5 had a single slope. This would
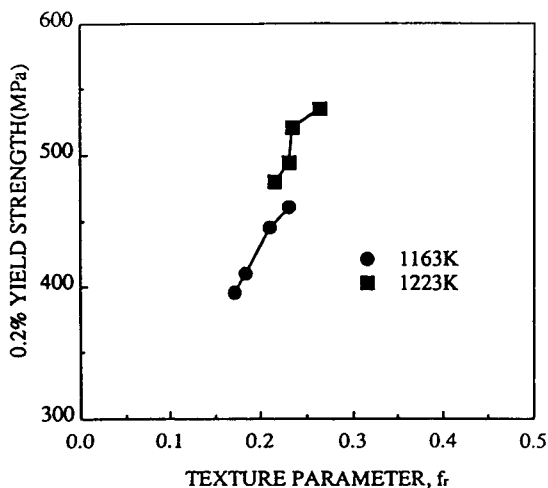

Fig. 5. Variation of the 0.2% Yield Strength with f_r.

suggest that the role of texture on the 0.2% yield strength was the same at both heat treatment conditions.

4. Discussion

4.1 Texture transformation

The factors relevant to the texture transformations during the $(\alpha + \beta)$ heat treatment would be kinetics of phase transformation and grain growth in the $(\alpha + \beta)$ phase filed.

The volume fraction of transformed β ($f_{\alpha'}$) was 0.20 and 0.58 for 5min at 1163K treatment and at 1223K, respectively, and 0.43 and 0.91 for 30min at both temperatures [16]. The observed textures were similar for 5min at 1163K and at 1223K as shown in fig. 2(a) and fig. 3(a), and also for 30min at both temperatures(fig. 2(b) and fig. 3(b)). This would suggest that the texture transformations were not much influenced by the volume fraction of transformed β phase. It is valid when the β transforms back to α by growth on the previous α grains keeping the same texture during the $(\alpha + \beta)$ heat treatment.
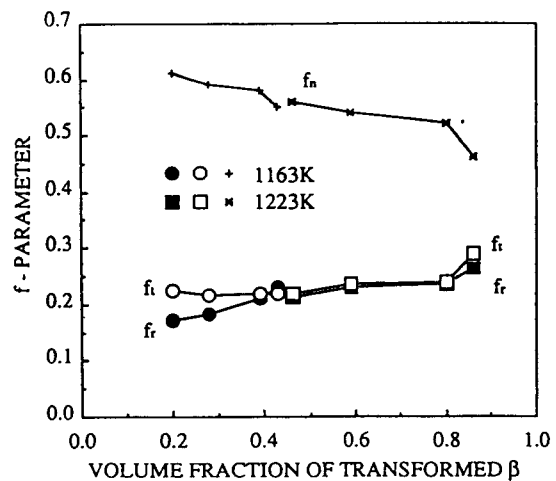

Fig. 6. Plot of f-Parameters against the Volume Fraction of Transformed β Phase.

On the contrary, the textures in the $(\alpha + \beta)$ phase field largely influenced the textures observed at room temperature. The inherited textures were similar to that of the α–annealed when the specimens were heat treated for 5min at both temperatures, however, it was true only when the texture in the $(\alpha + \beta)$ phase region did not develop by grain growth of the α or β phase grains which was the dominant factor introducing the preferred orientation in the metals [20].

Fig. 7 shows the plot of the prior $(\alpha + \beta)$ phase grain size against heat treating time. It can be seen that the grain growth kinetics obeys the empirical relationship $\bar{d} = kt^{\tau}$ given by Beck et al. [21], where $\bar{d}$ is average diameter(μm) of prior ($\alpha + \beta$) grains(μm), k is a constant, t is the heat treating time(sec), and τ is the time exponent of grain growth. The values for k and τ were found to be 8.8 and 0.14 at 1163K treatment, and 10.3 and 0.15 at 1223K. A small grain growth at both temperatures resulted in minor texture changes after the $(\alpha + \beta)$ heat treatment.

When the specimens were heat treated for 30min at both temperatures, the prior $(\alpha + \beta)$ grain size became twice as large as that of the α –annealed as shown in fig. 7. Although the Bur-
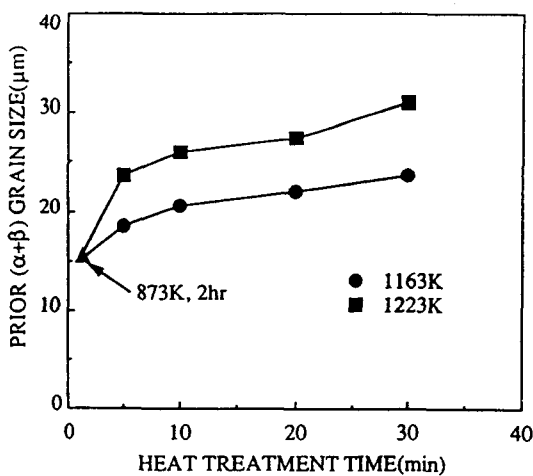

Fig. 7. **Plot of Prior $(\alpha + \beta)$ Grain Size against Heat Treatment Time.**

gers [10] relationship was still valid in the $\alpha \rightarrow \alpha + \beta$ transformation, the initial orientation relationships between α and β phase grains would differ to a large extent due to the grain growth of β phase grains. Then, the reorientation of basal poles from the normal–transverse plane of the sheet to the rolling–transverse plane was taken place on quenching from the $(\alpha + \beta)$ phase field. And the observed textures became more isotropic as the significant grain growth occurred.

4.2 Effect of texture on 0.2% yield strength

In fig. 5, the small increase in f_r resulted in the large increase in the 0.2% yield strength of the ($\alpha + \beta$) treated samples. This increase was rather exceptional compared to the influence of texture on the deformation behavior of the α and β transformed zirconium alloys [12,13]. Thus, it is necessary to determine whether this increase in the 0.2% yield strength is dependent only on the texture changes or not.

The transformed texture would affect the 0.2% yield strength of the $(\alpha + \beta)$ heat treated Zircaloy–4 sheet. In most cases, tensile deformation along the rolling direction of Zircaloy–4 sheet would occur by the operation of $\{10\bar{1}0\} < 1\bar{2}10>$ prism slip [13,22,23]. To estimate the effect of crystallographic texture alone on the yield strength of Zircaloy–4, the Schmid orientation factors and the resolved shear stresses on the $\{10\bar{1}0\} < 1\bar{2}10 >$ prism slip and twinning system were derived in the single crystal analogue, and presented in the Appendix.

The Kearns texture parameter f_r^s in the rolling direction for a single grain is

$$f_r^s = \cos^2\Phi \qquad (3)$$

where Φ is the tilt angle between the c–axis and the rolling direction. When the direction of the applied stress is parallel to the rolling direction, Φ

is equal to ϕ . When the expression (cosδ sinδ) of eq. (a2) is taken to be 1/2 as an angle δ varies from 0 to 180°, the Schmid factor m_p for the prism slip(Appendix I.) becomes

$$m_p = \sin^2\phi \, \cos\delta\sin\delta$$

$$= (1 - f_r^s) / 2 \tag{4}$$

The applied stress σ_a for yielding varies as the polycrystalline Zircaloy–4 has $\overline{m}_p$, where $\overline{m}_p$ is the average of the orientation factors m_p.

$$\sigma_a = \tau_p^c / \overline{m_p}$$

$$= \sigma_p^c / (1 - f_r) \tag{5}$$

where $\sigma_p^c(\cong 2\tau_p^c)$ is the critical stree for the yielding of Zircaloy, and f_r is the f–parameter of the polycrystalline Zircaloy–4 in the rolling direction. The eq.(5) neglects the interactions between the aggregate. From the literature [24], σ_p^c was taken to be 330MPa for the 0.2% yield strength of Zircaloy–2. It has been well known that the difference in the yield strength between Zircaloy–2 and Zircaloy–4 was not noted. As f_r approaches unity, the grains become oriented with their (0001) basal poles parallel to the rolling direction.

Tensile deformation parallel to the <0001> direction resulted from $\{10\overline{1}2\}<01\overline{1}1>$ twinning. The 0.2% yield strength of the Zircaloy–2 is 470Mpa when tensile stress is applied on the < 0001> direction [24]. This suggests that the deformation system may change at a certain tilt angle ϕ. This value was estimated to be 40° at room temperature deformation as confirmed in fig. 8.

It is seen in fig. 8 that the 0.2% yield strength of Zircaloys increased with increasing texture factor f in the loading direction. From the work of Ballinger and Pelloux [13], the 0.2% yield strength with f_r of a cold–worked and stress–relieved(CW–SR) Zircaloy–2 was higher than that calculated by eq. (5). This was attributable mainly
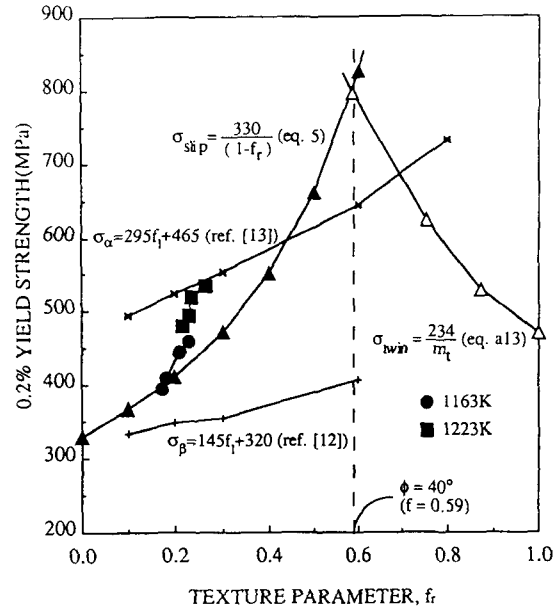

TEXTURE PARAMETER, f_r

Fig. 8. Variation of the 0.2% Yield Strength in Zircaloys with f_r.

to the microstructure of the CW–SR Zircaloy consisted of a deformed structure with partially recrystallized grains. Then, the large density of dislocations resulted in the higher yield strength of this alloy than that predicted by eq. (5).

In the case of β transformed Zircaloy [12], the yield strength with f_l(in longitudinal direction) was lower than that predicted by eq. (5). It was due to the recrystallization of the deformed structure and the formation of a coarse Widmanstätten α plate structure by β heat treatment. The soft Widmanstätten α plate might be easily deformed and this offset the increase of resolved shear stress as f_l increased. Then, the increase in the yield strength of β transformed Zircaloy–4 with increasing f_l became less than that predicted by eq. (5).

In the deformation of ($\alpha + \beta$) heat treated Zircaloy–4, the slight increase in f_r resulted in the sharp increase in the 0.2% yield strength. When compared with the case of the polycrystalline α and β transformed Zircaloys, the large increase in the yield strength with f_r would not be expected

from the small texture changes by the $(\alpha + \beta)$ heat treatment. It seemed rather to be influenced by the microstructural changes [16]. The $(\alpha + \beta)$ heat treatment gave rise to a mixture of hard primary α and soft transformed β structure. The accumulation of dislocations and the partitioning interfaces on quenching from the $(\alpha + \beta)$ phase temperature resulted in the rapid increase in the yield strength to a great extent. The 0.2% yield strength at the 1223K treatment was higher than that at the 1163K. It can also be attributed to the microstructural changes, which were greater at the 1223K treatment than that at the 1163K [16].

5. Conclusions

(1) The texture of α-annealed Zircaloy-4 sheet had the ideal orientation of the (0001) basal pole at $30°$ away from the normal direction toward the transverse direction. After the $(\alpha + \beta)$ treatment at 1163K and at 1223K, the observed textures were similar to the α-annealed texture when the prior $(\alpha + \beta)$ grain size was slightly larger than that of the α-annealed. However, the location of maximum basal pole intensity was distributed between the transverse and the rolling direction making an angle $15°$ from the normal direction, and the observed texture became more isotropic when the prior $(\alpha + \beta)$ grain size became twice as large as that of the α-annealed.

(2) It was found that the Kearns texture parameter, f_r in the rolling direction increased steadily, and f_t in the transverse direction increased slightly, while f_n in the normal direction decreased with increasing heat treatment time. The tendency for reorientation of the (0001) basal pole became more prevalent in the samples where a significant grain growth occurred during the $(\alpha + \beta)$ heat treatment.

(3) The 0.2% yield strength increased rapidly with increasing texture number, f_r. The large increase in the 0.2% yield strength with f_r was attri-

buted mainly to the microstructural changes by the $(\alpha + \beta)$ heat treatment. The role of texture on the yield strength was rather small, and it was confirmed by deriving the Schmid orientation factors and the resolved shear stresses for prism slip and twins in the single crystal analogue.

6. Acknowledgements

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Appendix

I. Derivation of the Schmid factor m_p and the resolved shear stress for the $|10\bar{1}0|$ $<1\bar{2}10>$ prism slip

In fig. Al, if we let X, Y, and Z be the three orthogonal coordinate axes in the α(hcp) Zircaloy–4 single crystal, then Z axis coincide with the [0001] axis. When the applied stress σ_a exerts on the single grain making an angle ϕ to the Z–axis and assuming that an angle between the trace of (Z–σ_a)-plane and X–axis is δ, the direction cosines between σ_a and Y–axis become as follows :

$$\cos\alpha = \sin\phi\cos\delta$$

$$\cos\beta = \sin\phi\sin\delta \tag{a1}$$

Then, the Schmid orietation factor m_p on $(01\bar{1}0)$ $[\bar{2}110]$ prism slip plane becomes

$$m_p = \cos\alpha\cos\beta$$

$$= \sin^2\phi \cos\delta\sin\delta \tag{a2}$$
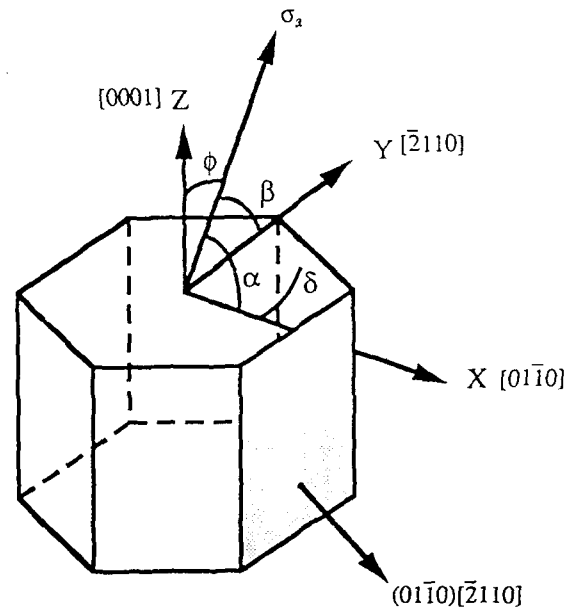

Fig. Al. Schematic Diagram of Hexagonal Crystal for $|12\bar{1}0|$ $<1\bar{2}10|$ Prism Slip.

and the resolved shear stress on this plane is

$$\tau_p = m_p \sigma_a$$
$$= \sigma_a \sin^2\phi \cos\delta \sin\delta \qquad (a3)$$

By the symmetry of the hexagonal structure, the range of angles $0 \leq \phi \leq 90°$ and $0 \leq \delta \leq 180°$ is satisfactory.

II. Derivation of the Schmid factor m_t and the resolved shear stress for the $\{10\bar{1}2\} < 0\bar{1}\bar{1}1 >$ tensile twin

Except for the crystallography of the twinned structures, the process of mechanical twinning is not clearly understood so far as the nucletion and growth of twins are concerned. For the homogeneous nucleation of twins one may use an expression similar to the slip process to estimate the critical resolved shear stress [al] ;·

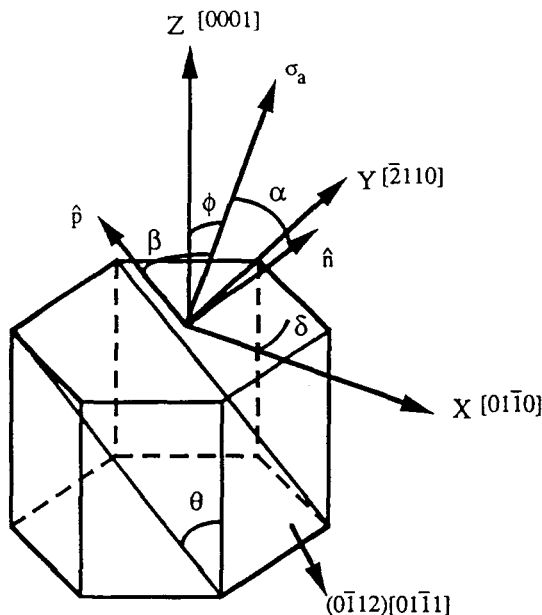$$C.R.S.S. \text{ for twinning} = K_t \frac{\gamma}{2\pi} \qquad (a4)$$

Fig. A2. Schematic Diagram of Hexagonal Crystal for $\{10\bar{1}2\} < 0\bar{1}\bar{1}1 >$ Tensile Twin.

where K_t is the transformed shear modulus on the twin plane in the twinning direction and γ is the shear strain of the twinning process. In this section, the orientation dependent stress nesessary for twinning is estimated by assuming that a twin will occur when the resolved shear stress on the twin plane reaches the C.R.S.S. for twinning, like a slip process.

In fig. A2, letting X, Y, and Z be the three orthogonal coordinate axes in hcp structure, then Z-axis coincides with the [0001] axis. The $\hat{i}$, $\hat{j}$, and $\hat{k}$ are the unit vectors along the X-, Y-, and Z-axes. It is assumed that $\hat{n}$ is the unit vector along the $(0\bar{1}12)$ twin plane normal, and $\hat{p}$ is the unit vector along the $[0\bar{1}\bar{1}1]$ twin direction in this twin plane. The, $\hat{p}$ becomes

$$\hat{p} = -\hat{i} \sin\theta + \hat{k} \cos\theta \qquad (a5)$$

where θ is the angle between the Z-axis and the $(0\bar{1}12)$ plane. The vector $\hat{n}$ can be found from the equation of twin plane, $Ax + By + Cz + D = 0$, in the XYZ-space. This equation contains the four lattice points, $(-\frac{\sqrt{3}}{2}a, \pm\frac{a}{2}, 0)$, and $(+\frac{\sqrt{3}}{2}a, \pm\frac{a}{2}, -c)$, where a and c are the lattice parameters of the hcp Zircaloy-4. Then, B, C and D become as follows :

$$A, B = 0, C = \frac{\sqrt{3} a}{c} A, \text{ and } D = \frac{\sqrt{3} a}{2} A \qquad (a6)$$

The unit vector $\hat{n}$ is

$$\hat{n} = (1, 0, \frac{\sqrt{3} a}{c}) / \sqrt{1 + (\frac{\sqrt{3} a}{c})^2} \qquad (a7)$$

When the applied stress σ_a exerts making ϕ to the Z-axis and assuming that an angle between the trace of $(Z-\sigma_a)$-plane and X-axis is δ, it becomes

$$\sigma_a = |\sigma_a| \cdot \hat{S}, \qquad (a8)$$

where $\hat{S} = (\hat{i} \sin\phi\cos\delta + \hat{j} \sin\phi\sin\delta + \hat{k} \cos\phi)$, the unit direction vector of σ_a. If it is assumed that an

angle between $\hat{n}$ and $\hat{S}$ is α, and an angle between $\hat{p}$ and $\hat{S}$ is β, then the orientation factor m_t for the tensile twin becomes as follows :

$$m_t = \cos\alpha\cos\beta \tag{a9}$$

where $\cos\alpha =$

$$\hat{n} \cdot \hat{S} = \frac{\sin\phi\cos\delta + \frac{\sqrt{3}\,a}{c}\cos\phi}{\sqrt{1 + (\frac{\sqrt{3}\,a}{c})^2}} , \tag{a10}$$

$$\cos\beta = \hat{p} \cdot \hat{S} = - \sin\theta\sin\phi\cos\delta + \cos\theta\cos\phi \tag{a11}$$

, or,

$$m_t = \frac{(\sin\phi\cos\delta + \frac{\sqrt{3}\,a}{c}\cos\phi)(- \sin\theta\sin\phi\cos\delta + \cos\theta\cos\phi)}{\sqrt{1 + (\frac{\sqrt{3}\,a}{c})^2}} \tag{a12}$$

Then, the resolved shear stress on this plane is

$$\tau_t = m_t \, \sigma_a \tag{a13}$$

In fig. A3, the maximum values of the orientation factors m_p and m_t are plotted against the tilt angle ϕ.
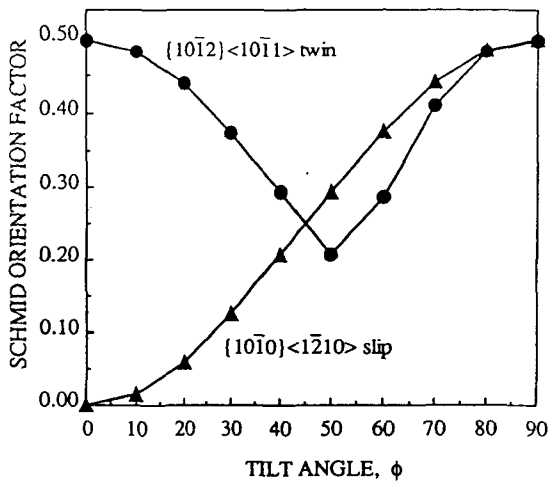

Fig. A3. Orientation Dependence of Schmid Factors for Slip and Twinning Systems in the hcp(α) Zircaloy–4.

Reference

[a1] Man Hyong Yoo and Chuan–Tseng Wei, Phil. Mag. 19 (1966) 573.