

FEA

NiAl

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A Study on the Orientation Dependence of Plastic Deformation in NiAl Single Crystals by FEA

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Key Words : Single crystal(), FEA(), Orientation dependence()

Abstract

Deformation of single crystals was studied using finite element analysis to investigate the orientation dependence of plastic deformation observed in NiAl single crystals. Investigation of mechanical properties of single crystals is closely related with the understanding of deformation processes in single crystals. Orientation dependence of material behavior in NiAl single crystals was studied by rotating loading directions from 'hard' orientation. The maximum nominal compressed stress in NiAl single crystals was ranged in a quite wide scope depending on the misalignment from 'hard' orientation. As the compressed axis set closer to 'hard' orientation, the maximum nominal compressed stress rapidly increased and made <100> slips difficult to activate. Therefore, non-<100> slips will be activated instead of <100> slips for 'hard' orientation.

1. , NiAl (Miracle, 1993, Winton, 1995).
 NiAl <100>
 가 (Brunner, D. and Gumbsch, P., 2001, Messerschmidt et al., 1997). orientation) ('hard'
 'soft' orientation)
 (grain boundary) NiAl
 가 NiAl 2 (kinematics),
 (constitutive equation) ABAQUS
 UMAT (user material subroutine)
 , 3 NiAl
 . 4

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2.

(constitutive model)

(rate dependent model)
1983, Peirce et al., 1983).

2.1

(deformation gradient)

(Lee, 1969).

$$\mathbf{F} = \mathbf{F}^* \cdot \mathbf{F}^p$$

, \mathbf{F}^*

\mathbf{F}^p

(slip system)

$\mathbf{s}^{(\alpha)}$

$\mathbf{m}^{(\alpha)}$

(orthogonal)

$\mathbf{s}^{(\alpha)}$ $\mathbf{m}^{(\alpha)}$

(convect)

$\mathbf{s}^{*(\alpha)}$

$\mathbf{m}^{*(\alpha)}$

$$\mathbf{s}^{*(\alpha)} = \mathbf{F}^* \cdot \mathbf{s}^{(\alpha)} \text{ and } \mathbf{m}^{*(\alpha)} = \mathbf{m}^{(\alpha)} \cdot (\mathbf{F}^*)^{-1} \quad (2.1)$$

(total velocity gradient) \mathbf{L}

(rate of stretching) \mathbf{D}

(rate of spin) $\mathbf{\Omega}$

(decompose)

$$\mathbf{L} = \dot{\mathbf{F}} \cdot \mathbf{F}^{-1} = \dot{\mathbf{F}}^* \cdot \mathbf{F}^{*-1} + \mathbf{F}^* \cdot \dot{\mathbf{F}}^p \cdot \mathbf{F}^{p-1} \cdot \mathbf{F}^{*-1} \quad (2.3)$$

$$\mathbf{L} = \mathbf{D} + \mathbf{\Omega} = \mathbf{L}^* + \mathbf{L}^p \quad (2.4)$$

, \mathbf{L}^*

, \mathbf{L}^p

가

$$\mathbf{L}^p = \mathbf{D}^p + \mathbf{\Omega}^p = \sum_{\alpha=1}^n \dot{\gamma}^{(\alpha)} (\mathbf{s}^{*(\alpha)} \cdot \mathbf{m}^{*(\alpha)\top}) \quad (2.5)$$

, $\dot{\gamma}^{(\alpha)}$

α

(shearing rate)

\mathbf{D}^p

(spin) $\mathbf{\Omega}^p$

$$\mathbf{D}^p = \sum_{\alpha=1}^n \dot{\gamma}^{(\alpha)} \cdot \mathbf{P}^{(\alpha)} \text{ and } \mathbf{\Omega}^p = \sum_{\alpha=1}^n \dot{\gamma}^{(\alpha)} \cdot \mathbf{W}^{(\alpha)} \quad (2.6)$$

$$\mathbf{P}^{(\alpha)} = \frac{1}{2} (\mathbf{s}^{(\alpha)} \cdot \mathbf{m}^{(\alpha)} + \mathbf{m}^{(\alpha)} \cdot \mathbf{s}^{(\alpha)})$$

$$\mathbf{W}^{(\alpha)} = \frac{1}{2} (\mathbf{s}^{(\alpha)} \cdot \dot{\mathbf{m}}^{(\alpha)} - \dot{\mathbf{m}}^{(\alpha)} \cdot \mathbf{s}^{(\alpha)})$$

2.2

Jaumann rate of Kirchhoff

Hook

(elastic rate of

stretching) \mathbf{D}^*

$$\sigma^{\nabla*} = \mathbf{L} : \mathbf{D}^*$$

, \mathbf{L} 4

(elastic moduli)

Jaumann

rate of Kirchhoff $\sigma^{\nabla*}$

$$\sigma^{\nabla*} = \dot{\sigma} - \mathbf{\Omega}^* \cdot \sigma + \sigma \cdot \mathbf{\Omega}^* \quad (2.9)$$

, $\dot{\sigma}$ Kirchhoff

(material rate

of Kirchhoff stress)

$\mathbf{\Omega}^*$

(rate of

spin tensor)

(material)

Jaumann rate of Kirchhoff

$$\sigma^{\nabla} = \dot{\sigma} - \mathbf{\Omega} \cdot \sigma + \sigma \cdot \mathbf{\Omega} \quad (2.10)$$

Eq. (2.9) eq. (2.10)

$$\sigma^{\nabla*} - \sigma^{\nabla} = \sum \beta^{(\alpha)} \cdot \dot{\gamma}^{(\alpha)} \quad (2.11)$$

$$\beta^{(\alpha)} = \mathbf{W}^{(\alpha)} \cdot \sigma - \sigma \cdot \mathbf{W}^{(\alpha)}$$

$$\sigma^{\nabla} = \mathbf{L} : \mathbf{D} - \sum_{\alpha=1}^n \dot{\gamma}^{(\alpha)} \mathbf{R}^{(\alpha)} \quad (2.12)$$

$$\mathbf{R}^{(\alpha)} = \mathbf{L} : \mathbf{P}^{(\alpha)} + \beta^{(\alpha)}$$

(strain rate

dependent material) power law (Pan and Rice, 1983)

(slip rate)

(resolved shear stress)

$$\dot{\gamma}^{(\alpha)} = \dot{a}^{(\alpha)} \left[\frac{\tau^{(\alpha)}}{\tau_c^{(\alpha)}} \right] \left[\frac{\tau^{(\alpha)}}{\tau_c^{(\alpha)}} \right]^{(1/m)-1} \quad (2.13)$$

, m

(rate sensitivity), $\tau_c^{(\alpha)}$

(critical resolved

shear stress), $\dot{a}^{(\alpha)}$

(reference strain rate)

(shear rate) $\dot{\gamma}$

(2.13)

2.3

(strain rate dependent)

가

$$\tau_c^{(\alpha)} = g(\gamma^{(\alpha)}) \quad (2.14)$$

가
가
 $\tau_c^{(\alpha)}$ 가
(Hill, 1965).

$$\dot{\tau}_c^{(\alpha)} = \sum_{\beta=1}^n h_{\alpha\beta} |\dot{\gamma}^{(\beta)}| \quad (2.15)$$

(hardening moduli) $h_{\alpha\beta}$
(Hutchinson, 1970).

$$h_{\alpha\beta} = qh + (1-q)h\delta_{\alpha\beta} \quad (2.16)$$

, q (latent hardening ratio)
(hardening rate) h
(critical resolved shear stress) $\tau_c(\gamma)$

(Peirce et al., 1983).

$$\tau_c(\gamma) = \tau_0 + (\tau_s - \tau_0) \tanh\left(\frac{h_0\gamma}{\tau_s - \tau_0}\right) \quad (2.17)$$

$$h(\gamma) = \frac{d\tau_c}{d\gamma} = h_0 \operatorname{sech}^2\left(\frac{h_0\gamma}{\tau_s - \tau_0}\right) \quad (2.18)$$

)

Schmid factor

(localization)

Levit et al. (1996) $[\bar{5}57]$

NiAl $\{110\}\langle 001\rangle$

$[\bar{5}57]$

(single slip)

eq. (2.17)

(monotonic)

(flow stress) (saturated) 가

(numerical parametric study)

(τ_0, τ_s, h_0)

τ_0, τ_s, h_0

Table 1

Table 1 Parameters used in the hardening curve

τ_0 (MPa)	τ_s (MPa)	h_0 (MPa)	m
26	38	110	0.04

, τ_0 (initial critical resolved shear stress), τ_s , (saturated shear stress), h_0 (initial hardening rate), m (strain rate sensitivity)

3. NiAl

NiAl

$\langle 100\rangle$

(‘hard’ orientation) (‘soft’ orientation) NiAl

$\{100\}\langle 001\rangle$

(resolved shear stress) 0

$\langle 111\rangle$ $\langle 110\rangle$

(Miracle, 1993).

(multi -slip activations) 가 NiAl

(idealized model)

$\{110\}\langle 001\rangle$

$\{100\}\langle 001\rangle$

(stereographic projection triangle) (misalignment)

$[001]$ - $[111]$

$[111]$

$\{110\}\langle 001\rangle$

(single slip)

(misalignment)

$[001]$ -

$[101]$

$[101]$

$\{100\}\langle 001\rangle$

(double slip)

(localized deformation)

(kinkband) 가

22

mm, 5 mm,

2 mm

(plane stress) 가

(Fig. 1).

(flange)

(flange)

가

(imperfection)

eq. (3.1)

Table 2

(Tvergaard et al., 1981).

$$\Delta h_0 = h_0 \left(-\bar{\xi}_1 \cos\left(\frac{\pi y}{L_0}\right) + \bar{\xi}_2 \cos\left(\frac{m\pi y}{L_0}\right) \right) \quad (3.1)$$

Table 2 material properties used in the simulation

	K (MPa)	G (MPa)		$\bar{\xi}_1$	$\bar{\xi}_2$	m
value	164916	68660	0.3221	0.0126	0.072	5

, K , G
 ABAQUS incompatible
 CPS4I 가
 (equivalent displacement rate)

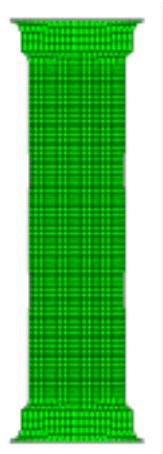


Fig. 1 Specimen used in the simulation

3.1 [001]-[111]

NiAl

(misalignment) [001]-[111]
 [111] {110}<001>
 (single slip)

([001]) (slip direction)

가

54.7

(kink

band) (border angle) 가 [001] 17

(border angle) ($\theta >$

17°) (monotonic) 가

(Fig. 2).

(Winton, 1995, Mielec et al., 1997).

가

(Fig.3-a, $\theta = 20^\circ$).

(border angle)

($3^\circ <$

$\theta < 17^\circ$)

(monotonic)

가

(Fig.2).

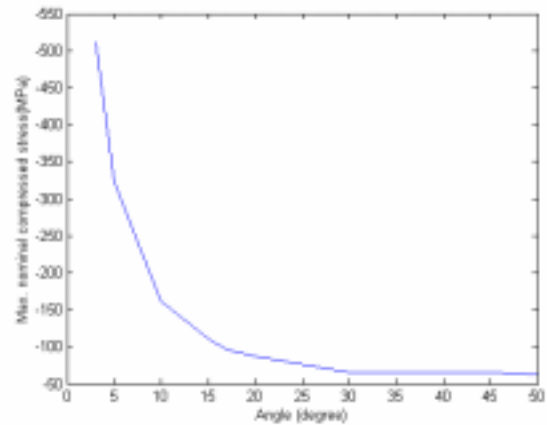


Fig. 2 Variations of the maximum nominal compressed stress with angle θ from [001] direction for single-slip case

(hard orientation)

가

가 (Fig. 2).

(Fraser et al., 1973a, Mielec et al., 1997)

가 (Fig.3-b,c, $\theta = 17^\circ, 5^\circ$).

60

(lattice rotation)

(Fig. 4)

(Fraser et al., 1973).

Fraser et al.

가

{110}<001>

60

Fig 5.

(kink band) 가

(single load drop)

(kink band)

3.2 [001]-[101]

NiAl

(misalignment) [001]-[101]

[101] (100)[010], (010)[100]

(double slip)

Fraser et al. (1973 a, b)

(kink band)

(compression axis)

<100>

1993) (Miracle,
 (double slip)
 (slip direction)
 45 가
 (single slip) 가
 (border angle) 가
 (single slip) 가
 (border angle)

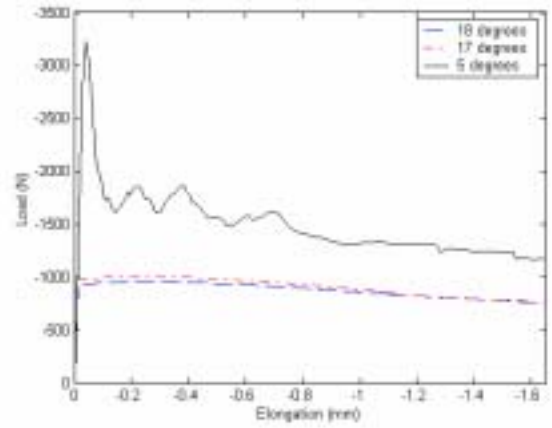


Fig. 5 Variations of the load with angle Θ for single-slip case

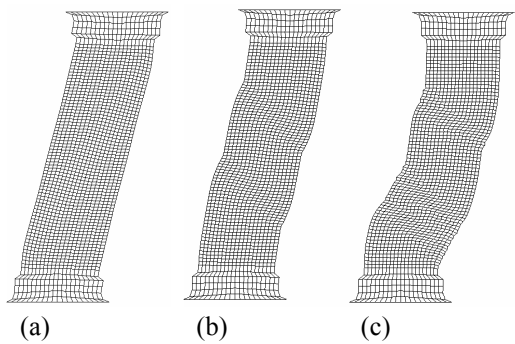


Fig. 3 Plots of deformed mesh with varying angle for single-slip case.
 (a) $\Theta = 20^\circ$ (b) $\Theta = 17^\circ$ (c) $\Theta = 5^\circ$

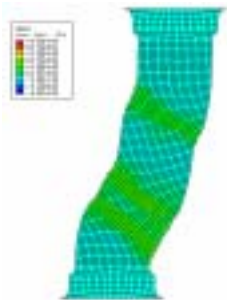


Fig. 4 Contour plots of lattice rotation with $\Theta = 5^\circ$ for single-slip case.

4.
 NiAl 가
 (kink band)
 (rotation softening)
 NiAl 가
 <100> 가
 <100> 가
 (double slip)
 [001]-[101] (kink band) [101]

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 (contract number: 2004-0101)
 BK21

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