Ab-initio calculation of the influence of Cr- and Ti-microalloying on the mechanical properties of NiAl

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Ab-initio calculations of material mechanical properties:

1. elastic constants
2. tensile test simulations
3. crack mechanics:
   (a) brittle crack; Griffith criterion
   (b) ductility - crack blunting; Rice concept of competition between brittle crack growth or dislocation emission
   (c) dislocation core properties, Peierls stress; Peierls-Nabarro model of dislocation

Competition between crack growth and dislocation emission

Stress intensity at the tip of the atomically sharp crack could lead to cleavage decohesion (brittle fracture) or dislocation emission (ductile fracture).

Actual fracture mode of given material can be found by comparation of *critical energy release rates* G of both processes.[1]

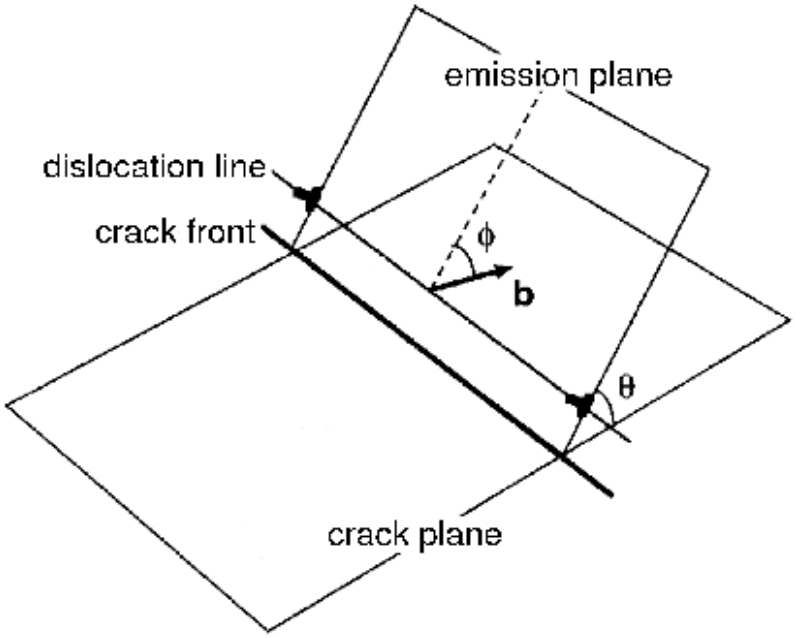
I. Griffith cleavage decohesion, critical energy release rate for cleavage:

$$G_c = 2\gamma_s$$

[1] J. Rice, *J. Mech. Phys. Solid.* **40**, (1992)

II. Dislocation emission from the tip, crack is blunted by one atomic plane, material tends to be ductile; a new material parameter - unstable stacking fault energy γ_{us} - is introduced

$$G_d = 8\frac{1+(1-\nu)\tan^2(\phi)}{1+\cos(\theta)\sin^2(\theta)}\gamma_{us}$$



Peierls-Nabarro model of dislocation

Dislocation is contructed by separating a crystal into two halves, adding one atomic plane into upper half and rejoining. Disregistry $f(x)$ between two half-planes is given by a balance between stress around dislocation and atomic restoring forces.

Restoring forces:

1. Frenkel model - forces are sinusoidal functions of disregistry and fulfil Hooke's law for small displacements. Solution is then

$$f(x) = -\frac{b}{2\pi} \arctan \frac{x}{\omega}$$

2. Forces are taken from stacking fault energy γ_{SF} surface

$$F(f(x')) = -\frac{\partial \gamma_{SF}(f(x'))}{\partial x'}$$

Solution with general forces - Lejček's method[2] : PN equation is taken as Hilbert transformation and so it may be written

$$\frac{df}{dx} \equiv \rho(x) = \sum_{k=1}^{N} \sum_{n=1}^{p_k} \rho_{nk}(x)$$

and restoring force

$$\frac{2\pi(1-\nu)}{\mu} \frac{\partial \gamma_{SF}(f(x))}{\partial x} = \sum_{k=1}^{N} \sum_{n=1}^{p_k} g_{nk}(x)$$

where

$$\rho_{nk} = \frac{1}{2} \left[\frac{A_{nk}}{(x - z_k)^n} + \frac{A^\star}{(x - z_k^\star)^n} \right]$$

$$g_{nk} = \frac{-i}{2} \left[\frac{A_{nk}}{(x - z_k)^n} - \frac{A^\star}{(x - z_k^\star)^n} \right]$$

This functions are fitted to a calculated γ_{SF} surfaces.

[2] L. Lejček, *Czech. J. Phys.* B **26**, (1976)

Why NiAl?

1. low density, high melting point, high strength
2. wide range of stability in atomic composition
3. site occupancy probability of additions can be varied by chemical composition[3]
4. BUT - poor ductility at room temperature

[3] Hao et al., *Mat. Sci. Eng.* **A365** (2004)

Methodology of the calculations

All calculations were performed using VASP (Vienna Ab-initio simulation package), which implements Projected Augmented Waves (PAW) method

I. Surface energy γ_s: crystal is "cut" into two halves, which are then separated. Energy as a function of separation distance x was fitted with universal binding energy relation (UBER)[4]

$$E = 2\gamma_s(1 + \frac{x}{l}) \exp\left(-\frac{x}{l}\right)$$

II. Stacking fault energy γ_{SF} is energy necessary to shift one half of the crystal against another (in given direction on the slip plane). Large supercell was used to exclude interaction between faults and positions of layers perpendicular to a slip were relaxed.

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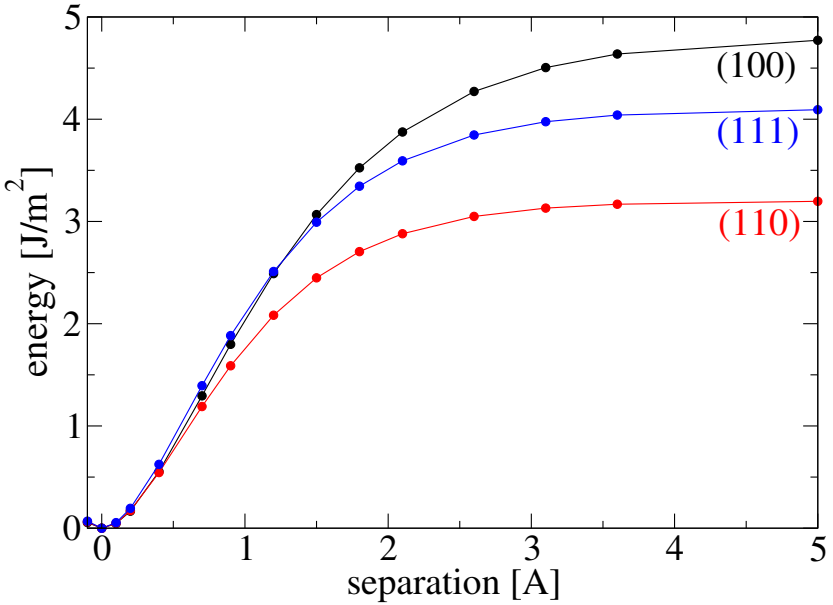
[4] Rose et al. *Phys. Rev.* B **28** (1983)

Cleavage properties



	G_c [J/m^2]	l [Å]	$\sigma[GPa]$
(001)	4.8	0.69	26
(011)	3.2	0.54	22
(111)	4.1	0.58	26

Dislocation emission

Slip system	γ_{us} [J/m^2]	γ_s/γ_{us}
$\langle 100\rangle(001)$	1.52	1.05
$\langle 110\rangle(001)$	2.9	0.55
$\langle 100\rangle(011)$	1.28	1.25
$\langle 01\bar{1}\rangle(011)$	2.09	0.77
$\langle 11\bar{1}\rangle(011)$	0.83	1.93
$\frac{1}{2}\langle 1\bar{1}0\rangle(111)$	1.61	1.0

1. ratio γ_s/γ_{us} is small (ductile fracture should appear for $\gamma_s/\gamma_{us} > 3.6$), so cleavage-type crack propagation should be expected

2. the largest value was found for $\langle 11\bar{1}\rangle(011)$ slip, however experimental results show that this slip system is unlikely in NiAl[5]

[5] Noebe et al., *Int. Mater. Rev.*, **38** (1993)

Effect of Microalloying

-microalloying is simulated by substitution of one atom at the surface of the crack with given element; supercell consisting of 64 atoms for slips at (001) plane and 32 for (011) plane is used

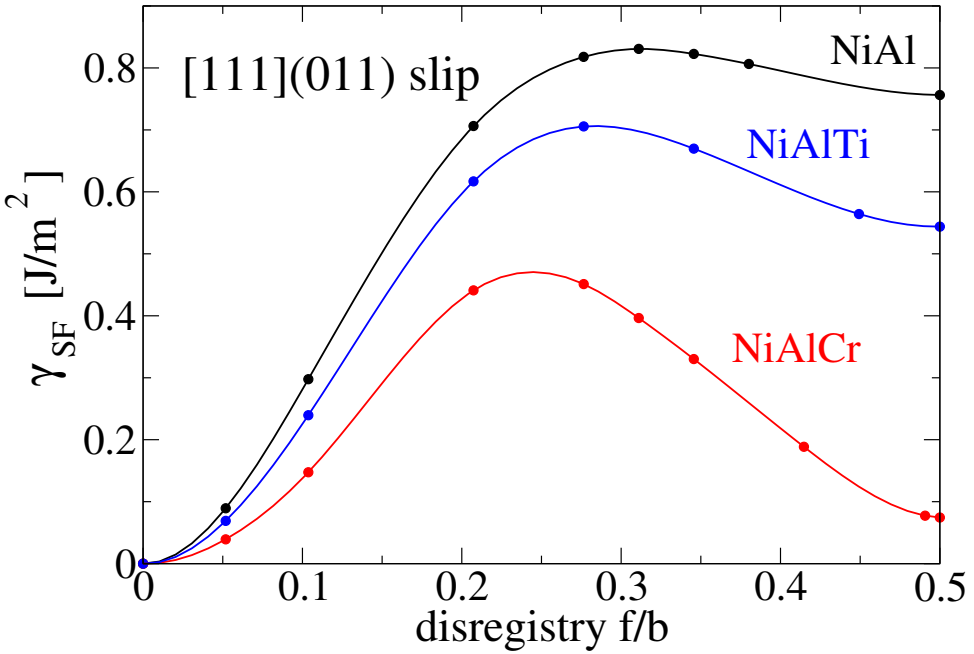
I. Effect on (001) layer properties

	pure NiAl	$Ni_{32}Al_{31}Cr$	$Ni_{31}Al_{32}Cr$
γ_s	2.9	2.9	2.98
$\langle 100 \rangle (001)$ slip	1.52	1.54	1.74
$\langle 110 \rangle (001)$ slip	2.9	-	3.34

	pure NiAl	$Ni_{32}Al_{31}Ti$	$Ni_{31}Al_{32}Ti$
γ_s	2.9	2.91	2.6
$\langle 100 \rangle (001)$ slip	1.52	1.54	1.42
$\langle 110 \rangle (001)$ slip	2.9	-	2.78

II. Effect on (011) layer properties

	pure NiAl	Ni_8Al_7Cr	Ni_8Al_7Ti
γ_s	1.6	1.94	1.63
$\langle 100 \rangle (011)$ slip	1.28	0.88	0.60

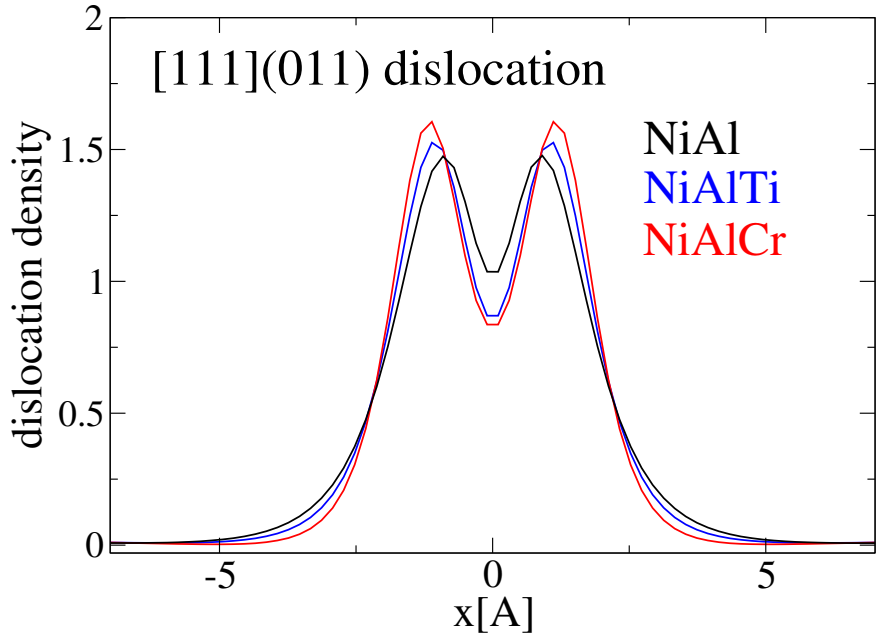


$\langle 11\bar{1}\rangle(011)$ dislocation properties

Forces derived from calculated γ_{SF}-surface were fitted with

$$\frac{2\pi(1-\nu)}{\mu}\frac{\partial\gamma_{SF}}{\partial f} = -\frac{b_{1k}}{(x-\delta_k)^2+\xi^2} - \frac{b_{2k}((x-\delta_k)^2-\xi^2)+2a_{2k}\xi(x-\delta_k)^2}{(x-\delta_k)^2+\xi^2}$$

and parameters were used to construct dislocation density.



Misfit energy and Peierls stress

Dislocation at position u - misfit e. $W(u) = a \sum_{m=-\infty}^{\infty} \gamma_{SF}(f(ma-u))$

For narrow dislocation only one plane contributes - $W(u) = a\gamma_{SF}(f(u))$

and stress can be calculated $\sigma(u) = \frac{1}{b}\frac{dW}{du}$

Its maximum is called Peierls stress $\sigma_p = \frac{a}{b} \max \left| \frac{\partial \gamma_{SF}(f)}{\partial f} \rho(u) \right|$

$\langle \mathbf{11\bar{1}} \rangle (\mathbf{011})$ dislocation	ξ/a	τ_{max}/μ	σ_p/μ
NiAl	0.22	1.0	0.049
NiAlCr	0.31	0.9	0.043
NiAlTi	0.24	0.72	0.049

Conclusions

1. NiAl found intrinsically brittle; main cleavage plane found is (011) in agreement with other calculations and experiments

2. the most promising slip system - $\langle 11\bar{1}\rangle(011)$ with $\gamma_s/\gamma_{us} = 1.93$ is not activated due to a very high Peierls stress, which also agrees with experimental results[6]

3. from various configurations checked, the most substantial effect has Cr-microallying to Al-positions for $\langle 11\bar{1}\rangle(011)$ slip; the γ_s/γ_{us} ratio increased to 3.6, but Peierls stress was not decreased enough to expect activation of this slip system

4. the prefered slip system found in experiments - $\langle 100\rangle(011)$ was more influenced by Ti-alloying but resulting γ_s/γ_{us} ratio of 2.7 still means cleavage fracture

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[6] Noebe et al., *Int. Mater. Rev.*, **38** (1993)

Outline for the future

1. More and more mechanical properties are accesible to ab-initio calculations; besides shown for example mobility of kinks[7], deformation twinning[8], interfacial dislocations[9] and many other

2. And even more problems are to be solved...

[7] Joos and Zhou, *Phil. Mag.* A, **81** 2001
[8] Tadmor and Hai, *J. Mech and Phys. Solids*, **51** 2003
[9] Yao and Wang, *Phys. Rev.* B, **59** 1999