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# On the core structure and mobility of the $\langle 100\rangle\{010\}$ and $\langle 100\rangle\{01\bar{1}\}$ dislocations in B2 structure YAg and YCu*

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Dislocations are thought to be the principal mechanism of high ductility of the novel B2 structure intermetallic compounds YAg and YCu. In this paper, the edge dislocation core structures of two primary slip systems $\langle 100\rangle\{010\}$ and $\langle 100\rangle\{01\bar{1}\}$ for YAg and YCu are presented theoretically within the lattice theory of dislocation. The governing dislocation equation is a nonlinear integro-differential equation and the variational method is applied to solve the equation. Peierls stresses for $\langle 100\rangle\{010\}$ and $\langle 100\rangle\{01\bar{1}\}$ slip systems are calculated taking into consideration the contribution of the elastic strain energy. The core width and Peierls stress of a typical transition-metal aluminide NiAl is also reported for the purpose of verification and comparison. The Peierls stress of NiAl obtained here is in agreement with numerical results, which verifies the correctness of the results obtained for YAg and YCu. Peierls stresses of the $\langle 100\rangle\{01\bar{1}\}$ slip system are smaller than those of $\langle 100\rangle\{010\}$ for the same intermetallic compounds originating from the smaller unstable stacking fault energy. The obvious high unstable stacking fault energy of NiAl results in a larger Peierls stress than those of YAg and YCu although they have the same B2 structure. The results show that the core structure and Peierls stress depend monotonically on the unstable stacking fault energy.

**Keywords:** YAg, YCu, core structure, Peierls stress
**PACC:** 6170G, 6155F, 6220

## 1. Introduction

The physical and mechanical properties of B2 structure (CsCl-type structure) intermetallic compounds, such as the transition-metal aluminides, have attracted much attention due to their high strength, high melting temperature, low density and good corrosion resistance for elevated temperature engineering applications.[1,2] However, the lack of ductility often severely limits the application of these intermetallic compounds at ambient temperature. In 2003, a new type of stoichiometric and ductile intermetallic systems was discovered by Gschneidner *et al.*[3−5] These alloys with B2 structure can be denoted as RM, where R is a rare-earth element and M is a late transition metal or an early p-element. Although the similarity of the crystal structure between RM and aluminides (such as NiAl), these intermetallics exhibit pronounced differences in their ductility behaviour. Much theoretical and experimental work has been done to reveal the mechanism of the ductility in these intermetallics in order to improve it in others.[6−9] Morris *et al* showed that the bonding in RM compounds is less covalent and less directional than that in NiAl.[10] This implies that the energy will change little in RM when the system is deformed in comparison with NiAl. A fundamental understanding of the ductile deformation of various materials is supplied by dislocation theory. To the knowledge of the authors, the core structure and Peierls stress of dislocations in the novel B2 structures YAg and YCu have not been reported in the literature. Thus, it is necessary to investigate the core structure of dislocations and the corresponding Peierls stress in RM compounds.

The Peierls–Nabarro (PN) model combined with the concept of generalized stacking fault energy (GSFE) has been extensively used to determine the dislocation core structure.[11−14] In the PN model the crystal is bisected along the glide plane into two semi-infinite half crystals which are treated as linear elastic continua. However, the continuous elastic treatment neglects the discreteness of the crystal, which is signif-

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icant to the core structure of dislocations as described in the lattice theory of dislocation.[15−18] As observed in experiments, the predominant slip systems in the typical RM compounds YAg and YCu are $\langle 100\rangle\{010\}$ and $\langle 100\rangle\{01\bar{1}\}$, which is in agreement with the predictions of dislocation theory.[4,19,20] In this paper, the core structure of the edge dislocations of $\langle 100\rangle\{010\}$ and $\langle 100\rangle\{01\bar{1}\}$ slip systems in YAg and YCu is determined within the lattice theory of dislocation. The variational method is applied to solve the modified PN equation due to its nonlinear integrodifferential character. The Peirels stress is calculated taking into account the contribution of elastic strain energy. The core width and Peierls stress of a typical transition-metal aluminide NiAl is also supplied for the purpose of comparison. The results show that the core width and Peierls stress are closely related to the unstable SFE.

## 2. Core structure of edge $\langle 100\rangle\{010\}$ and $\langle 100\rangle\{01\bar{1}\}$ dislocations

The modified PN dislocation related to the displacement of atoms on the border derived from lattice theory taking account of the lattice discreteness takes the following form:[15−18]

$$-\beta\frac{\mathrm{d}^2u}{\mathrm{d}x^2}-\frac{\mu\sigma}{\pi(1-\nu)}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x'}{x'-x}\Big(\frac{\mathrm{d}u}{\mathrm{d}x}\Big)\Big|_{x=x'}=f(u), \tag{1}$$

where $\sigma$ is the area of a primitive cell in a close-packed plane, and $\mu$ and $\nu$ are the shear modulus and Poisson ratio in the material. Comparing with the classical PN equation, we find that the modified PN equation (1) includes an extra term which is proportional to the second differential of the displacement field. The discreteness modification parameter $\beta$ describes the discrete effect of crystals and for edge dislocations

$$\beta=\frac{3}{4}\Omega\mu\bigg(\frac{2-2\nu}{1-2\nu}-\tan^2\theta\cos^2\phi\bigg), \tag{2}$$

where $\Omega$ is the volume of the primitive cell in the B2 structure, $\theta$ and $\phi$ are the orientation angles of the relative position of a pair of neighbouring atoms in the intrinsic frame with the axes given by the polarization directions. For disordered alloys, the B2 structure becomes equivalent to a body-centred cubic (bcc) lattice and the difference between atoms is neglected. Thus, $\theta=\arctan\sqrt{2}$ and $\phi=\pi/4$ for the $\langle 100\rangle\{010\}$ slip system and $\theta=\arctan(1/\sqrt{2})$ and $\phi=\pi/4$ for the $\langle 100\rangle\{01\bar{1}\}$ slip system. The restoring force $f(u)$ represents the nonlinear interaction on the bilateral of the slip plane. In the classic PN model, $f(u)$ takes a sinusoidal form and the approximation is very rough. Christian and Vitek suggested that the restoring force can be obtained from an effective interplanar potential, called the GSFE (or $\gamma-$surface).[21] The projections of atoms on the plane vertical to the dislocation line for $\langle 100\rangle\{010\}$ and $\langle 100\rangle\{01\bar{1}\}$ slip systems are shown in Fig.1. As shown in Fig.1, the GSFE curve

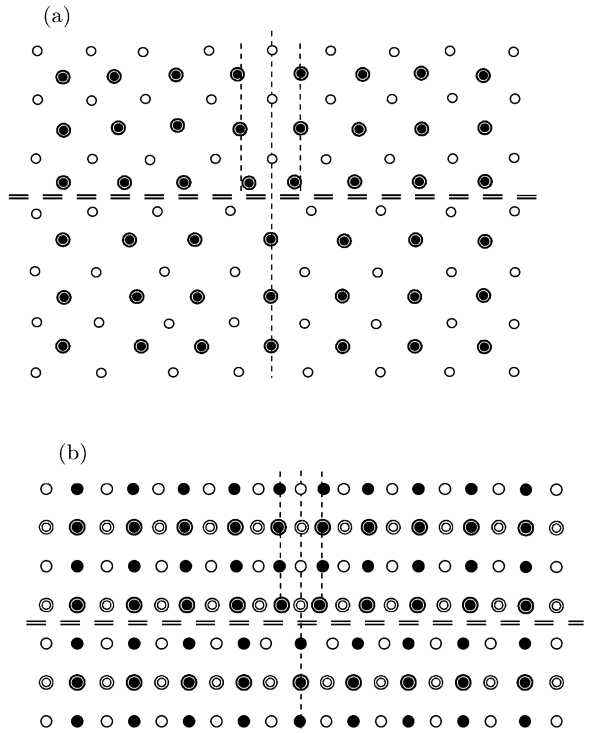



**Fig.1.** (a) The projection of atoms on the {001} plane due to edge dislocation of $\langle 100\rangle\{010\}$ slip system in the B2 structure. The double dashed line represents the slip plane. (b) The projection of atoms on the {011} plane due to edge dislocation of the $\langle 100\rangle\{01\bar{1}\}$ slip system in the B2 structure.

along the $\langle 100\rangle$ direction (double dashed line) possesses the periodicity due to the lattice and that can be expanded by Fourier series. Keeping the harmonic term, we have the modified sinusoidal force law

$$\gamma(u)=\frac{\mu b^2}{2\pi^2 d}\cos^2\Big(\frac{2\pi u}{b}\Big)\Big[1+\Delta\cos^2\Big(\frac{2\pi u}{b}\Big)\Big], \tag{3}$$

where $\Delta$ represents the modification of the sinusoidal force law, $b$ and $d$ are the Burgers vector and the interspacing between slip planes respectively. Equation (3) describes the GSFE curve well for the compact dislocation, $b$ equals the lattice parameter $a_0$, $d=a_0/2$ for the $\langle 100\rangle\{010\}$ slip system and $d=a_0/\sqrt{2}$ for the $\langle 100\rangle\{01\bar{1}\}$ slip system in the B2 structure. The

restoring force $f(u)$ can be deduced from the gradient of the GSFE curve, $f(u) = -\text{grad}\gamma(u)$. The corresponding restoring force of Eq.(3) can be obtained,

$$f(u) = \frac{\mu b}{2\pi d} \sin\left(\frac{4\pi u}{b}\right)\left[1 + 2\Delta\cos^2\left(\frac{2\pi u}{b}\right)\right]. \quad (4)$$

If $\Delta = 0$, Eq.(4) can be reduced to the sinusoidal force law. The profile of the unstable SFE and the restoring force for the ⟨100⟩{010} slip system of YAg, YCu and NiAl are plotted in Figs.2(a) and 2(b) respectively.

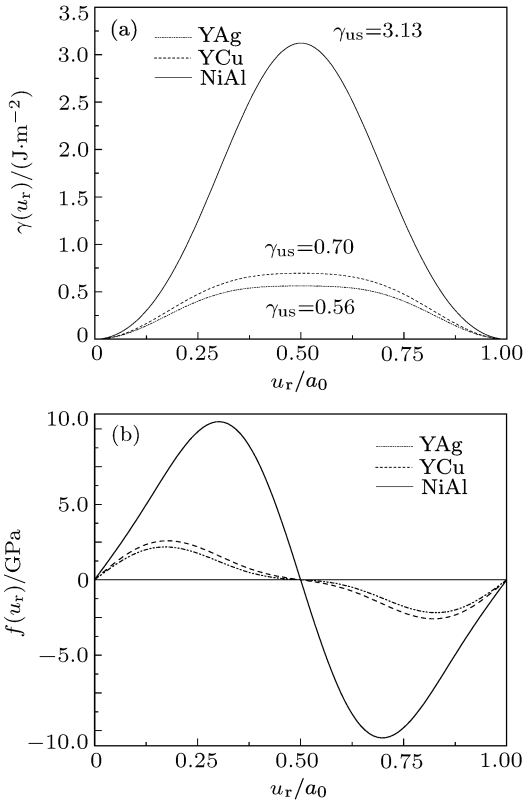



**Fig.2.** (a) The generalized stacking fault energy for the ⟨100⟩{010} slip system of YAg, YCu and NiAl modelled by Eq.(3). (b) The corresponding restoring force law of YAg, YCu and NiAl.

The Eq.(3) for GSFE is governed by the modification factor $\Delta$ or the the unstable stacking fault energy (USFE) $\gamma_{\text{us}}$ which is the maximum energy encountered in the block-like sliding along the Burgers vector in the slip plane

$$\gamma_{us} = (1 + \Delta)\frac{\mu b^2}{2\pi^2 d}. \quad (5)$$

The USFE $\gamma_{\text{us}}$ introduced by Rice is an important solid state parameter that characterizes the resistance to dislocation nucleation in materials.[22,23] While $\Delta = 0$, Eq.(5) denotes the simplest estimate of the unstable stacking fault energy based on the Frenkel sinusoid and $\gamma^0_{\text{us}} = \mu b^2/2\pi^2 d$. The $\Delta$ can be determined directly from Eq.(5) while the USFE is known and the required lattice constant, shear modulus and Poisson ratio are labelled in Table 1. Besides YAg and YCu, the quantities for NiAl are also given in Table 1 for comparison. The USFE of YAg, YCu and NiAl for the ⟨100⟩{010} and ⟨100⟩{01$\bar{1}$} slip systems are shown in Tables 2 and 3. The USFE, shear modulus, Poisson ratio and lattice parameter of RM and NiAl are taken from Refs.[10] and [14] respectively. The USFE of NiAl is much larger than that of YAg and YCu for the different bonding properties though they have the same crystal structure, and the difference also exists in the elemental metals.[10,24]

**Table 1.** The lattice constant $a_0$/Å, shear modulus $\mu$/GPa and Poisson ratio $\nu$ for YAg, YCu and NiAl.

| | $a_0$ | $\mu$ | $\nu$ |
|---|---|---|---|
| YAg | 3.634 | 28.2 | 0.32 |
| YCu | 3.477 | 34.2 | 0.29 |
| NiAl | 2.839 | 92.0 | 0.33 |

**Table 2.** The unstable stacking fault energy $\gamma_{\text{us}}/(\mathrm{mJ\cdot m^{-2}})$, modification factor $\Delta$, core width $\zeta(b)$ and Peirels stress $\tau_{\text{P}}(\mu)$ of ⟨100⟩{010} slip system for YAg, YCu and NiAl.

| | $\gamma_{\text{us}}$ | $\Delta$ | $c$ | $\zeta$ | $\tau_{\text{P}}$ |
|---|---|---|---|---|---|
| YAg | 560 | –0.46 | 0.83 | 2.12 | 0.0035 |
| YCu | 700 | –0.42 | 0.82 | 1.94 | 0.0058 |
| NiAl | 3130 | 0.67 | 0.71 | 1.38 | 0.0549 |

**Table 3.** The unstable stacking fault energy $\gamma_{\text{us}}/(\mathrm{mJ\cdot m^{-2}})$, modification factor $\Delta$, core width $\zeta(b)$ and Peirels stress $\tau_{\text{P}}(\mu)$ of ⟨100⟩{01$\bar{1}$} slip system for YAg, YCu and NiAl.

| | $\gamma_{\text{us}}$ | $\Delta$ | $c$ | $\zeta$ | $\tau_{\text{P}}$ |
|---|---|---|---|---|---|
| YAg | 315 | –0.57 | 0.86 | 3.58 | 0.000005 |
| YCu | 325 | –0.62 | 0.86 | 3.43 | 0.000012 |
| NiAl | 2280 | 0.19 | 0.78 | 2.45 | 0.0006 |

The dislocation equation (1) is a nonlinear integro-differential equation that is hard to solve. In the PN model, the method of residua in the complex plane introduced by Lejček is used to construct the dislocation core for an arbitrary form of the GSFE.[25] However, Eq.(1) with a second-order derivative term can no longer be considered as an example of a Hilbert transformation. Hereafter, the Ritz variational method is used to deal with the modified PN equation.[26] It can be easily verified that the variational functional of the dislocation equation takes the following form[26]

$$J=\frac{\beta}{2}\int_{-\infty}^{+\infty}\Big(\frac{\mathrm{d}u}{\mathrm{d}x}\Big)^2\mathrm{d}x-\frac{\mu\sigma}{2\pi(1-\nu)}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\frac{\mathrm{d}u}{\mathrm{d}x}\Big(\frac{\mathrm{d}u}{\mathrm{d}x}\Big)\Big|_{x=x'}\ln\Big|\frac{x-x'}{b}\Big|\mathrm{d}x\mathrm{d}x'+\frac{1}{2}\int_{-\infty}^{+\infty}\gamma(u)\mathrm{d}x. \quad (6)$$

The key step of the Ritz method is the selection of the trial function.[26] According to the structure character of the dislocation, the trial solution takes the following form

$$u(x)=\frac{b}{2\pi}\Big\{\arctan p+\frac{cp}{1+p^2}\Big\} \quad (7)$$

with $p=\kappa x$ and $\kappa=\kappa_0(1-c)$. In the region far from the dislocation core, the asymptotic behaviour of the trial solution is the same as the result obtained in continuum medium theory. For the edge dislocation, $\kappa_0=2(1-\nu)/d$. The core width of the dislocation is defined as the atomic spacing over which the relative displacement of the dislocation changes from $b/4$ to $3b/4$. The core width of the dislocation $\zeta$ is closely related to the parameter $c$ as revealed by Eq.(7). When we determine the parameter $c$, the core structure can be obtained expediently. It is instructive to note that $c$ contains the contribution of the modification of the sinusoidal force law and the effect of discreteness of the lattice. Obviously, the trial solution satisfies the boundary condition $u(x)|_{x\to\pm\infty}=\frac{b}{4}$.

Substituting the trial dislocation solution Eq.(7) into the variational functional Eq.(6), the variational functional $J$ is the function of parameter $c$ (the integral results of the three terms are given in Appendix A and for detailed derivation procedure, refer to Ref.[26]). The accurate position of the extremum of the functional is determined by the algebraic equation about $c$

$$\frac{\partial J}{\partial c}=0. \quad (8)$$

In Tables 2 and 3, $c$ and $\zeta$ for the $\langle100\rangle\{010\}$ and $\langle100\rangle\{01\bar{1}\}$ slip systems of YAg and YCu are listed. With the aim of comparison, $c$ and $\zeta$ of NiAl of the two slip systems are also presented. While both the discreteness of the lattice and the modification of the sinusoidal force law are neglected (viz. $\beta=0$ and $\Delta=0$), we have $c=0$ and core width $\zeta=\zeta_0=d/2(1-\nu)$. Taking the $\langle100\rangle\{010\}$ slip system of YAg as an example, the core width $\zeta_0=0.74b$. As shown in Table 2, $c=0.83$ and $\zeta=2.13b$ for $\Delta\neq0$ and $\beta\neq0$. In order to discuss the contribution of $\beta$ and $\Delta$ separately, we fix one of them to be zero. When $\beta=0$ and $\Delta=-0.46$ ($\gamma_{\rm us}<\gamma_{\rm us}^0$), the parameter $c=0.63$ and the core width $\zeta=1.12b$. If only the discreteness of the lattice is considered ($\beta\neq0$ and $\Delta=0$), the parameter $c=0.78$ and the core width $\zeta=1.70b$. Here, the results of the core structure of the $\langle100\rangle\{010\}$ slip system in NiAl is also given. $\zeta_0=0.75b$ for $\beta=0$ and $\Delta=0$. If only the effect of discreteness is considered ($\beta\neq0$ and $\Delta=0$), $c=0.78$ and the core width $\zeta=1.72b$. When both the modification of the sinusoidal force law and the effect of discreteness are taken into account $\beta\neq0$ and $\Delta=0.67$ ($\gamma_{\rm us}>\gamma_{\rm us}^0$), $c=0.71$ and the core width $\zeta=1.38b$. By comparing the core width of the $\langle100\rangle\{010\}$ slip system dislocation in YAg and NiAl labelled above, we can obtain the following conclusions: (i) the USFE $\gamma_{\rm us}>\gamma_{\rm us}^0$ ($\Delta>0$) leads to $\zeta<\zeta_0$ and $\gamma_{\rm us}<\gamma_{\rm us}^0$ ($\Delta<0$) results in $\zeta>\zeta_0$ when

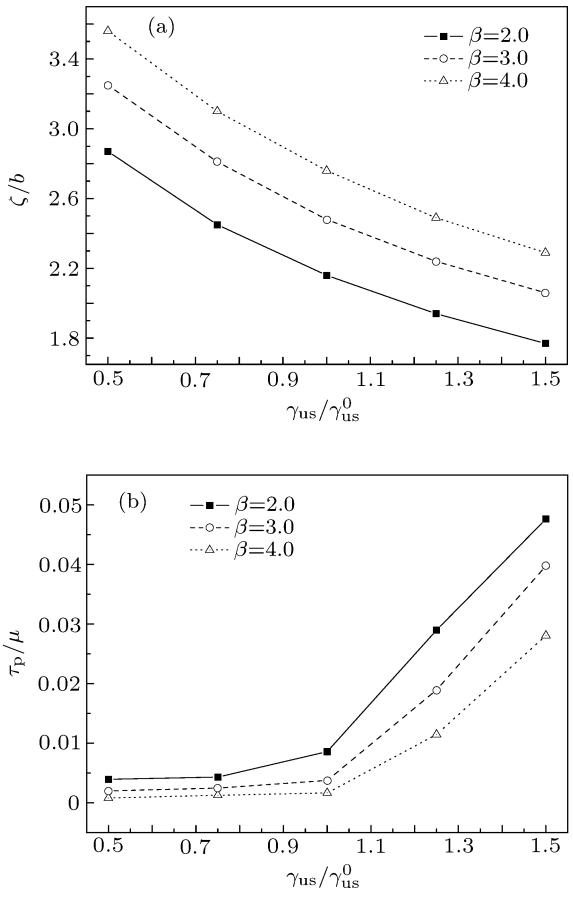



**Fig.3.** (a) The core width of dislocation $\zeta$ decreases monotonically with the increase of the unstable stacking fault energy $\gamma_{\rm us}$ for different discreteness modification factor $\beta$ (in units of $3\Omega\mu/4$). (b) Peierls stress $\tau_{\rm P}$ increases as the increasing of the unstable stacking fault energy $\gamma_{\rm us}$.

$\beta = 0$, (ii) the effect of lattice discreteness $\beta$ always makes the core structure wider than that obtained in the PN model. The core width of dislocations in NiAl is narrower than that in YAg and YCu due to the relatively high USFE $\gamma_{\rm us}$ as shown in Tables 2 and 3. In order to obtain the relation between the core width of the dislocation and the USFE, the USFE is endowed with different values and the plot for the ⟨100⟩{010} slip system of YAg is illustrated in Fig.3(a). The core width of dislocation $\zeta$ monotonically decreases as the increase of the USFE $\gamma_{\rm us}$. Furthermore, the larger the discreteness modification parameter $\beta$, the wider the core width of the dislocation.

## 3. Peierls stress of edge ⟨100⟩{010} and ⟨100⟩{01$\bar{1}$} dislocations

Peierls stress is the crucial quantity characterizing the mobility of dislocations that controls the mechanical properties of materials.[19] After the first estimation of the stress by Peierls and Nabarro, attempts to improve the prediction of the stress formula have been made within PN theory.[27−30] However, a long-standing contradiction—that the stable configuration of the dislocation has maximum energy rather than minimum energy—exists in PN theory.[31] It is found that the contradiction originates from the neglect of the contribution of the elastic strain energy, and only the misfit energy is considered in PN theory due to the continuous medium approximation. When the contribution of the elastic strain energy is taken into account, the contradiction is erased automatically.[31,32] The dislocation energy containing the contribution of the misfit energy and elastic strain energy associated with the discreteness of the lattice can be expressed as

$$E_{\rm dis}(l) = \sum_{n=-\infty}^{+\infty} \gamma[u(x_n - l)] + \sum_{n=-\infty}^{+\infty} f[u(x_n - l)]u(x_n - l), \quad (9)$$

where the first term and the second term are the misfit energy $E_{\rm mis}(l)$ and the elastic strain energy $E_{\rm ela}(l)$, respectively. $l$ is the position of the dislocation. The assumption of Nabarro is retained: that the profile of the dislocation core is independent of the position of the dislocation, namely, the dislocation moves rigidly.[28] In this paper, the dislocation energy possesses the following form

$$E_{\rm dis} = \sum_n \frac{\mu b^2}{2\pi^2 d}\cos^2\left(\frac{2\pi u_n}{b}\right)\left[1 + \Delta\cos^2\left(\frac{2\pi u_n}{b}\right)\right] + \sum_n \frac{\mu b}{2\pi d}\sin\left(\frac{4\pi u_n}{b}\right) \times \left[1 + 2\Delta\cos^2\left(\frac{2\pi u_n}{b}\right)\right]u_n. \quad (10)$$

When shifting rigidly along the slip direction, the dislocation energy varies periodically with the position $l$ of the dislocation centre. By means of the Poisson formula, the dislocation energy takes the following form:

$$E_{\rm dis}(l) = \frac{\mu b}{2\kappa\pi d}\sum_{n=-\infty}^{+\infty} A(n\xi)\mathrm{e}^{-\mathrm{i}n(\frac{2\pi l}{b} - \mathrm{i}\xi)}, \quad (11)$$

$$A(n\xi) = \frac{\mathrm{e}^{n\xi}}{\pi}\int_{-\infty}^{+\infty} f(\theta)\mathrm{e}^{\mathrm{i}n\xi p}\mathrm{d}p, \quad (12)$$

where

$$f(\theta) = (\cos^2\theta + \theta\cos\theta\sin\theta) + \Delta(\cos^4\theta + 2\theta\cos^3\theta\sin\theta) \quad (13)$$

with $\theta = 2\pi u/b$ and $\xi = 2\pi/\kappa b$.

Since $A(n\xi)$ is generally negligible for $|n| > 1$ when deducing the Peierls stress, we obtain

$$E_{\rm dis}(x) = \frac{\mu b}{2\kappa\pi d}A(0) + \frac{\mu b}{\kappa\pi d}A(\xi)\mathrm{e}^{-\xi}\cos\frac{2\pi x}{b}, \quad (14)$$

where $A(0)$ is a divergent constant associated with an infinite lattice.

Peierls stress is the minimum external stress to move a dislocation that can be obtained from the maximum slope of the dislocation energy

$$\tau_{\rm P} = \frac{2\mu}{\kappa d}|A(\xi)|\mathrm{e}^{-\xi}. \quad (15)$$

Peierls stress is crucially related with the kernel $A(\xi)$ that is obtained by the parametric derivation method in Ref.[32] and the final result of $A(\xi)$ is given in Appendix B.

Peierls stresses of YAg, YCu and NiAl for the ⟨100⟩{010} and ⟨100⟩{01$\bar{1}$} slip systems are given in Tables 2 and 3 respectively. The purpose of providing the Peierls stress of NiAl is to ensure the correctness of our calculations. For the dislocation of the ⟨100⟩{01$\bar{1}$} slip system, the Peierls stress $\tau_{\rm P}$ is equal to $0.0006\mu = 56$ MPa, which is in excellent agreement with the result obtained by the molecular static calculation 60 MPa.[33] The Peierls stress $\tau_{\rm P}$ is $0.0549\mu = 5047$ MPa for dislocation of the ⟨100⟩{010} slip system, which is in reasonable agreement with the order of magnitude of the numerical result supplied

by Schroll *et al.*[33] The Peierls stress of NiAl is larger than that of YAg and YCu for the dislocation of the same slip system. This is easy to understand since the USFE of NiAl is higher than that of YAg and YCu, and the USFE represents the highest barrier for a dislocation to surmount.[22,23] As illustrated in Fig.3(b), Peierls stress $\tau_{\rm P}$ increases monotonically with the increase of the USFE $\gamma_{\rm us}$. Thus, the mobility of dislocation and ductility of alloys can be modulated by alloying with variation of the SFE.[34,35] Furthermore, we can understand why Ag and Cu have approximately the same Peierls stress from the viewpoint that they have nearly the same USFE.[27,36] Thus, the USFE can be applied to predict the mobility of dislocations.

# 4. Conclusions

The core structure of edge dislocations in the $\langle 100\rangle\{010\}$ and $\langle 100\rangle\{01\bar{1}\}$ slip systems of B2 structure YAg and YCu are determined by the variational method taking into consideration the discreteness of the lattice. The USFE $\gamma_{\rm us} > \gamma_{\rm us}^0$ ($\Delta > 0$) leads to a narrow core and $\gamma_{\rm us} < \gamma_{\rm us}^0$ ($\Delta < 0$) gives a wide core where $\gamma_{\rm us}^0 = \mu b^2/2\pi^2 d$ denotes the simplest estimate of the USFE based on the Frenkel sinusoid. The discreteness modification parameter $\beta$ always leads to a wide core and the core width increases with the increase of $\beta$. Peierls stress is obtained following the procedure of Nabarro by combining the consideration of the contribution resulting from elastic strain energy. Peierls stress increases monotonically as the increase of the USFE. The core structure and Peierls stress of a typical transition-metal aluminide NiAl are also provided. The Peierls stress of NiAl $\tau_{\rm P}$ is in agreement with results obtained by numerical calculation. The Peierls stress of NiAl is larger than that of YAg and YCu, although they have the same B2 structure, due to the relatively higher USFE that can be deemed as the highest barrier for a moving dislocation to surmount.

# Appendix A

The integral results of the first two terms of Eq.(6) can be easily obtained by contour integration,

$$J_1 = \frac{\beta\kappa b^4}{16\pi}\Big(1 + c + \frac{c^2}{2}\Big), \tag{A1}$$

$$J_2 = \frac{\mu\sigma}{8\pi(1-\nu)}\Big[\ln\Big(\frac{\kappa b}{2}\Big) + c + \frac{c^2}{4}\Big]. \tag{A2}$$

The third term of Eq.(6) can be approximately obtained as

$$J_3 \approx \frac{\mu b^3}{8\pi\kappa d}\Big[(1+\Delta)\Big(2 - 2c + \frac{c^2}{2} + \frac{c^3}{6}\Big) - \frac{\Delta}{2}\Big(2 - 2c + \frac{c^2}{4} + \frac{c^3}{3} + \frac{c^4}{6}\Big)\Big]. \tag{A3}$$

Variational function $J = J_1 + J_2 + J_3$ is a function of parameter $c$.

# Appendix B

In order to obtain the kernel $A(\xi)$ more briefly, $f(\theta)$ may be rewritten into $f(\theta) = (f_{\rm mis} + f_{\rm ela}) + \Delta(f'_{\rm mis} + f'_{\rm ela})$ with $f_{\rm mis} = \cos^2\theta$, $f_{\rm ela} = \theta\cos\theta\sin\theta$, $f'_{\rm mis} = \cos^4\theta$ and $f'_{\rm ela} = 2\theta\cos^3\theta\sin\theta$. Accordingly, $A(\xi)$ can be separated into $A(\xi) = (A_{\rm mis} + A_{\rm ela}) + \Delta(A'_{\rm mis} + A'_{\rm ela})$. In Ref.[32], the parametric derivation method is applied and the results are

$$A_{\rm mis} = \frac{1}{2}\Big(2 + 2c\xi + \frac{3c^2\xi^2}{8} + \frac{5c^3\xi^3}{216}\Big), \tag{B1}$$

$$A_{\rm ela} = \frac{1}{2}(e_c + \ln(2\xi))\Big(-1 - c\xi - \frac{c^2\xi^2}{84} + \frac{c^3\xi^2}{6} - \frac{c^3\xi^3}{36}\Big), \tag{B2}$$

$$A'_{\rm mis} = \frac{1}{2}\Big(2 + 2\xi - 2c\xi + 2c\xi^2 - \frac{47c^2\xi^2}{24} + \frac{11c^2\xi^3}{18} - \frac{137c^3\xi^3}{216} + \frac{19c^3\xi^4}{216}\Big), \tag{B3}$$

$$A'_{\rm mis} = \frac{1}{2}(e_c + \ln(2\xi))\Big(-\xi + 2c\xi - c\xi^2 + \frac{7c^2\xi^2}{4} - c^3\xi^2 - \frac{c^2\xi^3}{3} - \frac{19c^3\xi^3}{36} - \frac{c^3\xi^4}{18}\Big), \tag{B4}$$

where $e_c = 0.5772\ldots$ is Euler constant.

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