IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

# The Peierls stress of the moving $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation in Ta

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2009 J. Phys.: Condens. Matter 21 345401

(http://iopscience.iop.org/0953-8984/21/34/345401)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 129.252.86.83
The article was downloaded on 29/05/2010 at 20:47

Please note that terms and conditions apply.

IOP Publishing Journal of Physics: Condensed Matter

J. Phys.: Condens. Matter **21** (2009) 345401 (5pp) doi:10.1088/0953-8984/21/34/345401

# The Peierls stress of the moving $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation in Ta*

**Ruiping Liu, Shaofeng Wang[1] and Xiaozhi Wu**

Institute for Structure and Function, Chongqing University, Chongqing 400044, People's Republic of China

E-mail: sfwang@cqu.edu.cn

Received 19 January 2009, in final form 14 June 2009
Published 28 July 2009
Online at stacks.iop.org/JPhysCM/21/345401

**Abstract**

The Peierls stress of the moving $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation with a planar and non-dissociated core structure in Ta has been calculated. The elastic strain energy which is associated with the discrete effect of the lattice and ignored in classical Peierls–Nabarro (P–N) theory has been taken into account in calculating the Peierls stress, and it can make the Peierls stress become smaller. The Peierls stress we obtain is very close to the experimental data. As shown in the numerical calculations and atomistic simulations, the core structure of the screw dislocation undergoes significant changes under the explicit stress before the screw dislocation moves. Moreover, the mechanism of the screw dislocation is revealed by our results and the experimental data that the screw dislocation retracts its extension in three {110} planes and transforms its dissociated core structure into a planar configuration. Therefore, the core structure of the moving $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation in Ta is proposed to be planar.

## 1. Introduction

It is generally accepted that the dislocations play a prominent role in controlling the properties of materials, in particular their mechanical behavior [1, 2]. Since the screw dislocation is considered to be of primary importance in controlling the plastic deformation of bcc crystals at low temperature, the core structure has been studied extensively by numerical calculations and atomistic simulations [3–5]. It is suggested by Hirsch that the screw dislocation can dissociate into more than one plane, and that such a non-planar dissociation can interpret the observed high Peierls barrier and the strong temperature dependence of the yield stress [6]. Although various different splittings of the screw dislocation were taken into account [7], with the help of computer simulations, the idea of the famous three-way dissociation into three equivalent {110} planes is widely accepted, that is, the core structure of the static screw dislocation is dissociated into three equivalent {110} planes. However, it is speculated whether the core structure of the screw dislocation is still dissociated into three equivalent {110} planes when the screw dislocation moves. Consequently, some numerical calculations and atomistic simulations were conducted, and it is shown that the core structure always undergoes significant changes under the explicit stress before the screw dislocation moves [8–11]. Then the core structure must retract some of its extension and transform to a different configuration, whereas the degree of retracting its extension is still undetermined. In order to get the core structure of the moving screw dislocation, the Peierls stress of the screw dislocation has been widely calculated by numerical calculations and atomistic simulations. However, there is still a discrepancy between the calculated results and experimental data in that the Peierls stress predicted by the numerical and atomistic simulations is much higher than that observed at low temperature. The previous simulations of the screw dislocation in Ta are around 1.5 GPa [12–14], whereas the experimental data is 260 MPa. Afterward, the Peierls stress obtained from the new model generalized pseudopotential theory (MGPT) [15, 16] and the qEAM2 force field [17] are about 660 and 440 MPa, respectively. The reason of the discrepancy may be the incomplete understanding of the mechanism of the dislocation motion, and the configuration of the core structure is very important to the Peierls stress when the screw dislocation moves.

* This work was supported by the National Natural Science Foundation of China (10774196), the Science Foundation Project of CQ CSTC (2006BB4156) and Chongqing University Postgraduates' Science and Innovation Fund (200707A1A0030240).

[1] Author to whom any correspondence should be addressed.

 © 2009 IOP Publishing Ltd Printed in the UK

In classical P–N theory, only the misfit energy is considered in calculating the dislocation energy. However, in the context of the full lattice theory, it is found that, except for the misfit energy, the extra elastic strain energy which is associated with the discreteness of the lattice is crucial to the dislocation energy, and it can make the dislocation energy become much smaller than that in classical P–N theory [18]. In this paper, the Peierls stress of the moving $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation with planar and non-dissociated core structure in Ta is calculated. By taking into account the elastic strain energy, the Peierls stress of the screw dislocation with planar core structure is about 200 MPa, and it is very close to the experimental data. Therefore, it can be speculated just as was shown in previous calculations that the core structure of the $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation undergoes significant changes under the explicit stress before the screw dislocation moves. Furthermore, the screw dislocation transforms its dissociated core structure in three {110} planes to a planar core structure. Therefore, the core structure of the moving $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation in Ta is proposed to be planar.

## 2. The modified P–N equation of the screw dislocation

The modified P–N equation due to the lattice discrete correction has been obtained firstly using the solvable models and derived later in a model-independent way [19–21], and the modified P–N equation of screw dislocation taking into account the discrete correction of lattice takes the following form:

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

where $u$ is the relative displacement of the bilateral misfit planes along the slip direction $\langle 111\rangle$, $\mu$ is the shear modulus in the direction $\langle 111\rangle$, $\beta$ is the parameter of the discrete correction of lattice to the core structure and $f$ is the nonlinear interaction which can be calculated from the generalized-stacking-fault (GSF) energy [22]. The parameter $\beta$ related to the acoustic phonon velocity and the lattice geometry structure [21] and $f$ can be given by

$$\beta=\frac{3}{4}\frac{\Omega\mu}{\sigma}(1-\tan^2\theta\sin^2\phi). \qquad (2)$$

$$f=-\frac{\partial\gamma}{\partial u} \qquad (3)$$

and

$$\gamma=\frac{\mu b^2}{2\pi^2 d}\sin^2\frac{\pi u}{b}\left(1+\Delta\sin^2\frac{\pi u}{b}\right), \qquad (4)$$

where $\Omega$ is the volume of the primitive cell, $\sigma$ is the area of the primitive cell of the misfit plane, $\theta$, $\phi$ are the orientation angles of the relative position of a pair of neighboring atoms in the intrinsic frame with the axes given by the polarization directions, $b=\sqrt{3}a/2$ is the Burgers' vector, $d=\sqrt{2}a/2$ is the spacing between misfit planes and $a$ is the lattice constant of the bcc crystals. For $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation, $\theta=\pi/4$, $\phi=\arcsin\sqrt{3}/3$, $a=3.30$ Å and $\mu=65.1$ GPa for Ta [23]. The dimensionless parameter $\Delta$ describes the higher-order corrections of the misfit energy in the Fourier series, and it can be determined by fitting the GSF energy in the direction $\langle 111\rangle\{110\}$. If $\Delta=0$, then the sinusoidal force law in the classical P–N model can be recovered.

**Table 1.** The values of the fitting parameter $\Delta$ of the GSF energies of Ta.

| | FP LMTO | VASP | MGPT | qEAM2 | qEAM3 |
|---|---|---|---|---|---|
| $\Delta$ | −0.270 | −0.344 | −0.360 | −0.373 | −0.422 |

The GSF energy in the direction $\langle 111\rangle\{110\}$ of Ta has been calculated by the MGPT potential, the full-potential linear muffin-tin orbital (FP LMTO) method [15], the first-principles-based force field (FF) qEAM1, qEAM2 and qEAM3 potentials [17] and the first-principles *ab initio* method (VASP—Vienna *ab initio* Simulation Package) [24]. Because the GSF energy from the FF qEAM1 agrees very well with FP LMTO, then FF qEAM1 is not considered here. In order to display the fitting effects, the fitted GSF energies from MGPT, FP LMTO and VASP have been plotted in figure 1 for example, and the values of $\Delta$ have been shown in table 1. It can be seen from figure 1 that the numerical results can be well described by equation (4) and $\Delta$ always takes the negative values as can be seen from table 1.

The modified P–N equation (1) can also be solved by the truncating method given by one of the authors previously [25]. The solution is

$$u=\frac{b}{\pi}\left[\arctan p+\frac{(1-\varepsilon)p}{1+p^2}\right]+\frac{b}{2}, \qquad (5)$$

with $p=\kappa x$ and $\kappa=\kappa_0\varepsilon=2\varepsilon/d$. After complicated calculations, an algebraic equation about $\Delta$, $\varepsilon$ and $\varepsilon_0$ can be obtained:

$$\Delta\left(\frac{10}{9}+\frac{\varepsilon}{3}\right)+(1-\varepsilon)^2-\frac{\varepsilon^2}{\varepsilon_0^2}\left(1-\frac{11\varepsilon}{16}\right)=0, \qquad (6)$$

and $\varepsilon$ is the root of the algebraic equation. The dimensionless parameter $\varepsilon_0$ only depends on the elastic properties and geometry structure with

$$\frac{1}{\varepsilon_0^2}=\frac{8\beta}{\mu d}. \qquad (7)$$

For $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation, $\varepsilon_0=0.500$. The structure factors $\varepsilon$ and $\Delta$ obtained from fitting different GSF energies have been summarized in table 2. It is displayed by equation (6) that $\varepsilon$ is related to $\varepsilon_0$ and $\Delta$, that is, the structure factor $\varepsilon$ is determined by the discrete correction of the lattice and the modification of the sinusoidal force law, and it can be shown in table 3 that $\varepsilon$ increases with increasing $\Delta$.

## 3. The Peierls stress in classical P–N theory

In the classical P–N theory, only the misfit energy is considered in calculating the dislocation energy, and the Peierls stress can be written as [26]

$$\sigma_p=A\mathrm{e}^{-\frac{\alpha\xi}{b}}, \qquad (8)$$

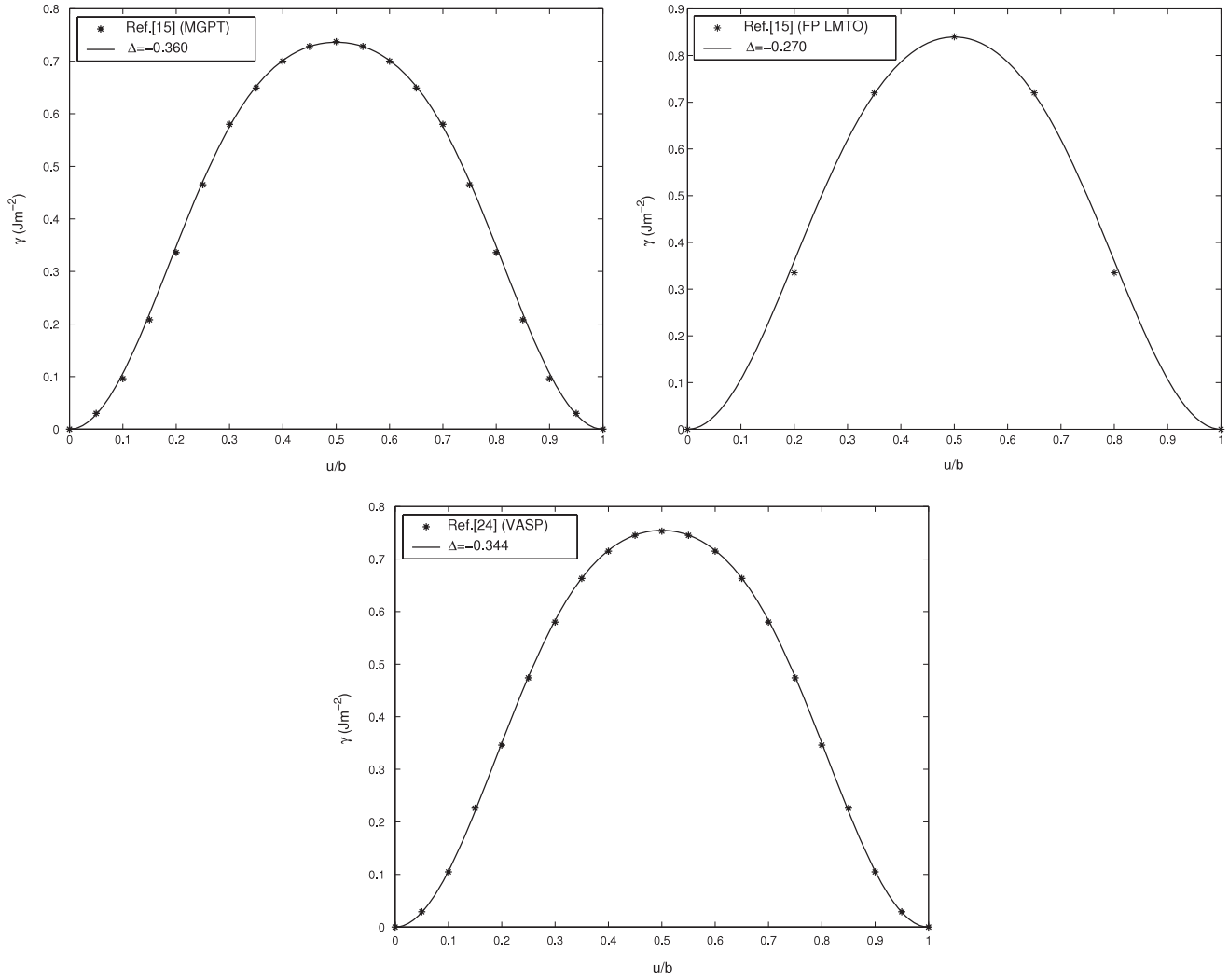


**Figure 1.** The fitting of the GSF energy. The solid lines and the stars represent the GSF energy used in this paper and calculated in other references, respectively.

**Table 2.** The values of $\varepsilon$ with FP LMTO, VASP, MGPT, qEAM2 and qEAM3 methods.

| | FP LMTO | VASP | MGPT | qEAM2 | qEAM3 |
|---|---|---|---|---|---|
| $\Delta$ | −0.270 | −0.344 | −0.360 | −0.373 | −0.422 |
| $\varepsilon$ | 0.261 | 0.232 | 0.226 | 0.221 | 0.202 |

**Table 3.** The Peierls stress of screw dislocation of Ta (in units of GPa) only considering the modification of the sinusoidal force law.

| | FP LMTO | VASP | MGPT | qEAM2 | qEAM3 |
|---|---|---|---|---|---|
| $\Delta$ | −0.270 | −0.344 | −0.360 | −0.373 | −0.422 |
| $\varepsilon$ | 0.419 | 0.350 | 0.336 | 0.326 | 0.286 |
| Peierls stress | 2.70 | 2.00 | 1.87 | 1.78 | 1.34 |

where $\alpha = 2\pi$, $\xi$ is the half-width of the dislocation. For $1/2\langle 111\rangle\{110\}$ screw dislocation, $A = \mu$, $\xi = 1/\kappa_0$ and the Peierls stress given by equation (8) is about 5 GPa ($7.69 \times 10^{-2}\mu$). It is obvious that the Peierls stress in classical P–N theory is very high. The possible reason is that the half-width of the screw dislocation is too narrow. Nevertheless, the discrete effect of the lattice can make the core width broaden [27]. Therefore, it is necessary to take into account the lattice discrete effect, and it is not approximate to calculate the dislocation energy and the Peierls stress using the classical P–N theory.

## 4. The Peierls stress of the $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation in bcc Ta

In the context of the full lattice theory, it is found that, besides the misfit energy, the elastic strain energy which is also associated with the discrete effect of the lattice is also crucial to the dislocation energy, and the dislocation energy can be written as [18, 28]

$$E = E_{\text{mis}} + E_{\text{ela}}, \tag{9}$$

where $E_{\text{mis}}$ is the misfit energy, $E_{\text{ela}}$ is the elastic strain energy and the Peierls stress can be obtained from the maximum slope of the dislocation energy. If the elastic strain energy and the discrete correction as well as the modification of the sinusoidal

**Table 4.** The Peierls stress of screw dislocation of Ta (in units of MPa) as well as the corresponding $\Delta$ and $\varepsilon$.

| | FP LMTO | VASP | MGPT | qEAM2 | qEAM3 | Experiments |
|---|---|---|---|---|---|---|
| $\Delta$ | −0.270 | −0.344 | −0.360 | −0.373 | −0.422 | — |
| $\varepsilon$ | 0.261 | 0.232 | 0.226 | 0.221 | 0.202 | — |
| Peierls stress | 214 | 257 | 250 | 241 | 182 | 260 |

force law are not considered, then the Peierls stress is just that in P–N theory.

In order to investigate the effect of the elastic strain energy, lattice discrete correction and the modification of the sinusoidal force law to the Peierls stress, some calculations have been done using the parametric derivation method [28].

(i) Only taking into account the elastic strain energy without considering the discrete correction and the modification of the sinusoidal force law, that is $\Delta = 0$ and $\varepsilon = 1$, then the Peierls stress is about 532 MPa ($8.17 \times 10^{-3}\mu$). It is obvious that the elastic strain energy can make the Peierls stress become much smaller, being one order of magnitude smaller than that in the P–N model.

(ii) Only taking into account the discrete correction of the lattice without considering the discrete correction and the elastic strain energy, that is $\Delta = 0$, $\varepsilon = 0.366$, then the Peierls stress is 1.45 GPa ($2.22 \times 10^{-2}\mu$), which is smaller than that in the P–N model only in magnitude.

(iii) Only considering the modification of the sinusoidal force law without taking into account the discrete correction and the elastic strain energy, the corresponding $\varepsilon$ and the Peierls stress with $\Delta$ have been summarized in table 3. It is shown in table 3 that the modification of the sinusoidal force law can only make the magnitude of the Peierls stress in the P–N model become smaller.

In general, it can obviously be seen that the three factors of the elastic strain energy, the discrete correction and the modification of the sinusoidal force law can all make the Peierls stress become smaller, and the elastic strain energy is the most important for the Peierls stress. Therefore, it is indispensable to consider the elastic strain energy as well as the discrete correction and the modification of the sinusoidal force law in calculating the Peierls stress.

By taking into account the three factors above, we calculate the Peierls stress of the $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation with planar and non-dissociated core structure in Ta. The results we obtain have been shown in table 4. As can be seen, our results are around 200 MPa and they are very close to the experimental data of 260 MPa.

That the Peierls stress of the planar screw dislocation is very close to the experimental data indicates that the core structure may be planar when the $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation moves. It has been revealed by numerical calculations and atomistic simulations that the core structure of the screw dislocation always undergoes significant changes under the explicit stress before the screw dislocation moves [8–11]. Our results not only validate that fact but also can explain the possible mechanism of the screw dislocation motion. It is shown that, under the explicit stress, just the same as in the prediction of the numerical calculations and atomistic simulations, the screw dislocation undergoes significant changes. Furthermore, it retracts the extension in three {110} planes and transforms its dissociated core structure into a planar configuration. Obviously, the planar core structure is much easier to move than the dissociated core structure in three {110} planes. Despite the core structures of the moving $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocations in other bcc metals are not always planar, at least it is proposed to be planar in Ta.

Initially, the Peierls stress obtained from the numerical calculations in Ta is about 1.5G Pa, which is several times of the experimental data of 260 MPa. This value is much lowered in recent numerical simulations. The Peierls stress obtained from the new MGPT potential and the qEAM2 force field is about 660 and 440 MPa, respectively. With the further improvement of the atomistic potentials and the calculation precision, the Peierls stress may be decreased further and closer to the experimental data.

## 5. Summary

The Peierls stress of the moving $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation with planar and non-dissociated core structure in Ta has been calculated. The elastic strain energy which is associated with the discrete effect of the lattice and ignored in classical P–N theory has been taken into account in calculating the Peierls stress. The Peierls stress we obtain is very close to the experimental data. It is revealed by the Peierls stress of the planar screw dislocation and the experimental data as well as the prediction of the numerical calculations and the atomistic simulations that, under the explicit stress, the core structure of the screw dislocation undergoes significant changes. Furthermore, it retracts its extension in three {110} planes and transforms its dissociated core structure into a planar configuration before the screw dislocation moves. Therefore, the core structure of the moving $\frac{1}{2}\langle 111\rangle\{110\}$ screw dislocation in Ta is proposed to be planar.

## References

[1] Hirth J P and Lothe J 1982 *Theory of Dislocations* 2nd edn (New York: Wiley)
[2] Schoeck G 2005 *Mater. Sci. Eng.* A **400** 7–17
[3] Cottrell A H and Bilby B A 1951 *Phil. Mag.* **42** 573
[4] Cohen J B, Hinton R, Lay K and Sass S 1962 *Acta. Metall.* **10** 894
[5] Frank F C and Nicholas J F 1953 *Phil. Mag.* **44** 1213
[6] Hirsch P B 1960 *5th Int. Conf. on Crystallography* Cambridge University p 139
[7] Vitek V 1974 *Cryst. Lattice Def.* **5** 1
[8] Basinski Z S, Duesbery M S and Taylar R 1971 *Can. J. Phys.* **49** 2160–80

Basinski Z S, Duesbery M S and Taylar R 1971 *Interatomic Potentials and Simulation of Lattice Defects, Battele Colloquium* ed P C Gehlen *et al* (New York: Plenum) pp 537–52
[9] Duesbery M S, Vitek V and Bowen D K 1973 *Proc. R. Soc.* A **332** 85–111
[10] Vitek V 1976 *Proc. R. Soc.* A **352** 109
[11] Rao S I and Woodward C 2001 *Phil. Mag.* A **81** 1317–27
[12] Wang G F, Strachan A, Cağin T and Goddard W A 2001 *Mater. Sci. Eng.* A **309/310** 133–7
[13] Woodward C and Rao S I 2002 *Phys. Rev. Lett.* **88** 216402
[14] Ito K and Vitek V 2001 *Phil. Mag.* A **81** 1387
[15] Yang L H, Söderlind P and Mariarty J A 2001 *Phil. Mag.* A **81** 1355–85
[16] Moriarty J A, Belak J F, Rudd R E, Soderlind P, Streitz F H and Yang L H 2002 *J. Phys.: Condens. Matter* **14** 2825
[17] Wang G F, Strachan A, Cağin T and Goddard W A 2003 *Phys. Rev.* B **68** 224101
[18] Wang S F 2006 *Chin. Phys. Soc.* **15** 1301–9
[19] Wang S F 2002 *Phys. Rev.* B **65** 094111
[20] Wang S F 2008 *J. Phys. A: Math. Theor.* **41** 015005
[21] Wang S F 2009 *J. Phys. A: Math. Theor.* **42** 025208
[22] Wang S F, Wu X Z and Wang Y F 2007 *Phys. Scr.* **76** 593
[23] Simmon G and Wang H 1971 *Single Crystal Elastic Constants and Calculated Aggregate Properties: a Handbook* (Cambridge: MIT)
[24] Woodward C 2005 *Mater. Sci. Eng.* A **400/401** 59–67
[25] Wang S F 2003 *Phys. Lett.* A **313** 408
[26] Joós B and Duesbery M S 1997 *Phys. Rev. Lett.* **78** 266–9
[27] Wang S F, Liu R P and Wu X Z 2008 *J. Phys.: Condens. Matter* **20** 485207
[28] Wu X Z and Wang S F 2007 *Acta Mech. Solida Sin.* **20** 4