Available online at www.sciencedirect.com
ScienceDirect
Scripta Materialia 61 (2009) 355–358
Scripta MATERIALIA
www.elsevier.com/locate/scriptamat

Analysis of stress field of a screw dislocation inside an embedded nanowire using strain gradient elasticity

K.M. Davoudi,[a] M.Yu. Gutkin[b,c] and H.M. Shodja[a,d,*]

[a]Department of Civil Engineering, Center of Excellence in Structures and Earthquake Engineering, Sharif University of Technology, 11155-9313 Tehran, Iran

[b]Institute of Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoj 61, Vasil. Ostrov, St. Petersburg 199178, Russia

[c]Department of Physics of Materials Strength and Plasticity, St. Petersburg State Polytechnical University, Polytekhnicheskaya 29, St. Petersburg 195251, Russia

[d]Institute for Nanoscience and Nanotechnology, Sharif University of Technology, 11155-9161 Tehran, Iran

Received 20 March 2009; accepted 4 April 2009
Available online 12 April 2009

The stress field of a screw dislocation inside an embedded nanowire is considered within the theory of strain-gradient elasticity. It is shown that the stress singularity is removed and all stress components are continuous and smooth across the interface, in contrast with the results obtained within the classical theory of elasticity. The maximum magnitude of dislocation stress depends greatly on the dislocation position, the nanowire size, and the ratios of shear moduli and gradient coefficients of the matrix and nanowire materials.

Keywords: Strain gradient elasticity; Screw dislocation; Nanowire

Fabrication, characterization and application of embedded nanowires are among the hottest topics in materials science and applied physics. Nanowire-based structures and devices are developed for wide use in various fields of nanoscience (e.g. biology, electronics, medicine, optics, optoelectronics, photonics and sensors). It is well known that the structure and properties of embedded nanowires depend greatly on their environment. In particular, much attention has been paid to the elastic strains and stresses that arise in or near the embedded nanowires due to the presence of defects [1] and differences in the material properties of the nanowires and surrounding matrix [1,2]. The theoretical consideration of these questions is commonly based on the classical theory of elasticity; however, this cannot be applied to extremely (atomically) thin nanowires, interface areas and defect cores. There are two ways to overcome these limitations. The first is to discard the continuum description and use atomic simulations [3,4]. The second is to still exploit the continuum approach but within an extended theory of elasticity that could cope with classical difficulties (singularities, jump discontinuities, etc.). The theory of strain-gradient elasticity seems to be the most simple and effective extension of classical elasticity in this sense.

The governing equation of the simple isotropic theory of gradient elasticity proposed by Ru and Aifantis [5] reads

$$(1-\ell^2\nabla^2)\boldsymbol{\sigma} = (1-c^2\nabla^2)[\lambda(\mathrm{tr}\boldsymbol{\varepsilon})\mathbf{I} + 2\mu\boldsymbol{\varepsilon}] \tag{1}$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are the elastic stress and strain tensors, respectively, λ and μ are the Lamé constants, $\mathbf{I}$ is the unit tensor, ∇^2 is the Laplacian and $\ell, c \geqslant 0$ are two gradient coefficients (different in a general case) which represent intrinsic length scales within the gradient theory. It was strictly proved [5,6] that the solution of Eq. (1) boils down to the independent solution of the following inhomogeneous Helmholtz equations for the stress $\boldsymbol{\sigma}$ and displacement $\mathbf{u}$ fields:

$$(1-\ell^2\nabla^2)\boldsymbol{\sigma} = \boldsymbol{\sigma}^0 \tag{2}$$

* Corresponding author. Address: Department of Civil Engineering, Center of Excellence in Structures and Earthquake Engineering, Sharif University of Technology, 11155-9313 Tehran, Iran. Tel.: +98 21 66164209; fax: +98 21 66072555; e-mail: shodja@sharif.edu

1359-6462/$ - see front matter
doi:10.1016/j.scriptamat.2009.04.010

$$(1 - c^2\nabla^2)\mathbf{u} = \mathbf{u}^0 \quad (3)$$

where $\boldsymbol{\sigma}^0$ and $\mathbf{u}^0$ denote the corresponding fields calculated in the theory of classical elasticity. For a crystalline solid with the lattice parameter a, numerical estimates have been made for ℓ and c based on theoretical models [7–12] and experimental observations [13]. For example, Eringen [7,8] obtained Eq. (2) in his version of the theory of nonlocal elasticity and found that $\ell \approx 0.39a$. Altan and Aifantis [9] derived Eq. (3) and came up with $c \approx 0.25a$.

Eqs. (2) and/or (3) have been applied to the problems of dislocations [7,8,14–23], disclinations [20,24,25], cracks [5,6,9,26,27], composite materials [28], inclusions [29], line forces and the Flamant problem [30]. Some of these works were extensively reviewed in Refs. [31,32]. The main general result is the elimination of classical singularities from the solutions for elastic fields and energies. For dislocations placed near interphase boundaries, the image forces have also been regularized [17–19,23]. Moreover, it has been shown that in the problems for inclusions [29], dislocations inside free-surface nanowires [22] and outside embedded nanowires [23], the maximum values of elastic fields become size-dependent, in contrast with the corresponding classical solutions, which are size-independent. The aim of the present paper is to consider the elastic stress of a screw dislocation placed inside an embedded nanowire in the framework of the strain gradient elasticity described by Eqs. (1)–(3).

Let a screw dislocation lie at the point $(\xi, 0)$ inside an infinite cylinder (nanowire) Ω embedded in an infinite elastic medium (matrix) D (Fig. 1). In classical elasticity, this problem was solved in displacements by Dundurs [33]. The nonvanishing stress components yield (in units of $b/2\pi$) the following:

$$\sigma_{zx}^{0(D)} = -\mu_D(1+S)\frac{y}{r_1^2} + \mu_D S\frac{y}{r^2},$$

$$\sigma_{zy}^{0(D)} = \mu_D(1+S)\frac{x_1}{r_1^2} - \mu_D S\frac{x}{r^2},$$

$$\sigma_{zx}^{0(\Omega)} = -\mu_\Omega\frac{y}{r_1^2} + \mu_\Omega S\frac{y}{r_2^2}, \quad \sigma_{zy}^{0(\Omega)} = \mu_\Omega\frac{x_1}{r_1^2} - \mu_\Omega S\frac{x_2}{r_2^2}, \quad (4)$$

where b is the Burgers vector, μ_D and μ_Ω are the shear moduli of the matrix and the nanowire, respectively, $S = (\mu_\Omega - \mu_D)/(\mu_\Omega + \mu_D)$, $x_1 = x - \xi$, $x_2 = x - R^2/\xi$, R is the nanowire radius, $r^2 = x^2 + y^2$ and $r_{1,2}^2 = x_{1,2}^2 + y^2$. This solution clearly demonstrates limitations of the classical theory. First, near the dislocation line, when $r_1 \to 0$, the stress components $\sigma_{zx}^{0(\Omega)}$ and $\sigma_{zy}^{0(\Omega)}$ are singular. Secondly, the stress component $\sigma_{zr}^0 = \sigma_{zx}^0\cos\theta + \sigma_{zy}^0\sin\theta$ is continuous across the interface, $\sigma_{zr}^{0(D)}|_{r=R} = \sigma_{zr}^{0(\Omega)}|_{r=R} = -(\mu_D b/2\pi)(1+S)\ \xi\sin\theta/(R^2 - 2R\xi\cos\theta + \xi^2)$, and also becomes singular there when the dislocation reaches the interface ($\xi \to R,\ \theta = 0$). Thirdly, the stress component $\sigma_{z\theta}^0 = -\sigma_{zx}^0\sin\theta + \sigma_{zy}^0\cos\theta$ suffers an abrupt jump at the interface, $[\sigma_{z\theta}^0]_-^+ = \sigma_{z\theta}^{0(D)}|_{r=R} - \sigma_{z\theta}^{0(\Omega)}|_{r=R} = -(S/R)[\mu_D + \mu_\Omega(R^2 - \xi^2)/(R^2 - 2R\xi\cos\theta + \xi^2)]$, which depends on the dislocation position. When the dislocation approaches the interface ($\theta = 0, \xi \to R$), the stress jump, $[\sigma_{z\theta}^0]_-^+ \to -2\mu_\Omega S/(R-\xi)$, drastically increases and becomes singular. All these features make it impossible to use the classical solution (4) in the case of dislocations in atomically thin nanowires. As was discussed previously in detail [17,18], the stress jump at the interface, $[\sigma_{z\theta}^0]_-^+$, is justified in the classical theory of elasticity aimed at describing macroscopic elastic solids because it does not contribute to the traction vector that should be in balance at the interface. However, from the nanoscopic point of view, this assumption does not seem to be valid. Indeed, the stress jump is doubtful in view of the fact that atoms forming the interface interact with other atoms belonging to both the materials in contact. Hence, the assumption of a transitional region near the interface, where the interaction between atoms varies gradually from stronger in more rigid material to weaker in other materials, is unavoidable. It can be concluded from this assumption that the stress jump is only a consequence of the approximation of classical continuum models, which often become insufficient for describing nanoscale phenomena.

Let us consider the same problem within the gradient theory described by Eqs. (1)–(3). The full solution procedure and results for all elastic fields and image forces will be given elsewhere [34]. Here we concentrate on the main peculiarities of the gradient solution for stress field. Thus, the stress equation (2) must be solved for both regions D and Ω. Due to the existence of higher-order derivatives, some additional boundary conditions are needed. Following Refs. [17–19,23], we have used the following conditions of balance for stresses and stress gradients at the interface:

$$[\sigma_{zr}]_-^+ = 0, \quad [\sigma_{z\theta}]_-^+ = 0, \quad \left[\frac{\partial\sigma_{zr}}{\partial r}\right]_-^+ = 0, \quad \left[\frac{\partial\sigma_{z\theta}}{\partial r}\right]_-^+ = 0. \quad (5)$$

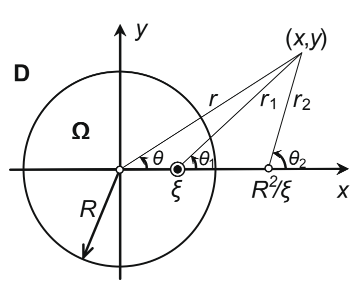

Figure 1. A screw dislocation inside an embedded nanowire.

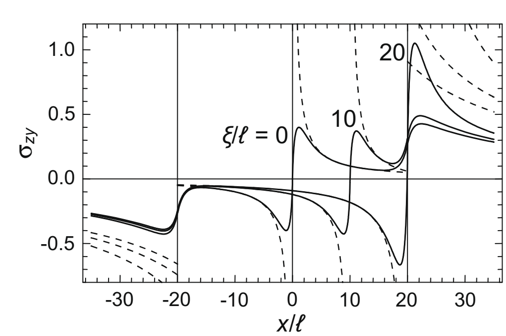

Figure 2. The stress component $\sigma_{zy}(x, 0)$ of a screw dislocation placed at the position $\xi/\ell_\Omega = 0$, 10, and 20 in the case of $R = 20\ell_\Omega$, $\mu_D/\mu_\Omega = 10$, and $\ell_\Omega = \ell_D$. Solid and dashed curves correspond to the gradient and classical solutions, respectively. The stress values are given in units of $\mu_\Omega b/(2\pi\ell_\Omega)$.

Here $[]^+_-$ denotes the difference in the corresponding quantity across the interface. These conditions can be a remedy for the unrealistic classical stress jump (see above) and provide a continuous and smooth transition of the stress field through the interphase boundary. With Eqs. (5), the gradient solution reads

$$\sigma_{zx}^{(D)} = \sigma_{zx}^{0(D)} + \mu_D(1+S)y\Phi(r_1;\ell_D) - \mu_D S y \Phi(r;\ell_D) + \sum_{n=1}^{\infty} B_n K_n\left(\frac{r}{\ell_D}\right)\sin n\theta,$$

$$\sigma_{zx}^{(\Omega)} = \sigma_{zx}^{0(\Omega)} + \mu_\Omega y\Phi(r_1;\ell_\Omega) - \mu_\Omega S y \Phi(r_2;\ell_\Omega) + \sum_{n=1}^{\infty} b_n I_n\left(\frac{r}{\ell_\Omega}\right)\sin n\theta,$$

$$\sigma_{zy}^{(D)} = \sigma_{zy}^{0(D)} - \mu_D(1+S)x_1\Phi(r_1;\ell_D) + \mu_D S x_1 \Phi(r;\ell_D) + \sum_{n=1}^{\infty} A_n K_n\left(\frac{r}{\ell_D}\right)\cos n\theta,$$

$$\sigma_{zy}^{(\Omega)} = \sigma_{zy}^{0(\Omega)} - \mu_\Omega x_1\Phi(r_1;\ell_\Omega) + \mu_\Omega S x_2 \Phi(r_2;\ell_\Omega) + \sum_{n=0}^{\infty} a_n I_n\left(\frac{r}{\ell_\Omega}\right)\cos n\theta, \qquad (6)$$

where the first terms are the classical stress components given by Eqs. (4), I_n and K_n denote the modified Bessel functions of the first and second kind, respectively, of order n, and $\Phi(r;\ell) = bK_1(r/\ell)/(2\pi\ell r)$. The unknown coefficients A_n, a_n, B_n and b_n are easily determined from the boundary conditions (5); however, they are so cumbersome that we do not present them here.

The gradient solution (6) is free from the classical limitations. The appearance of the modified Bessel function $K_1(r_1/\ell_\Omega)$, which has the asymptotic $\sim\ell_\Omega/r_1$ at $r_1 \to 0$, eliminates the stress singularity at the dislocation line (Fig. 2). This cancels the two first limitations of the classical solution mentioned before. Moreover, both the stress components, σ_{zr} and $\sigma_{z\theta}$, are continuous and smooth across the interface (for example, see Fig. 2 for $\sigma_{zy} = \sigma_{z\theta}$ at $\theta = 0$), thus deleting the third limitation. As a result, the gradient solution for the image force on dislocation, $F_x(\xi) = b_z\sigma_{zy}^{(\Omega)}(x=\xi,\ y=0)$, becomes finite everywhere, in contrast with its classical solution, which is infinite at the interface. The gradient solution (6) turns to the classical solution (4) in the limits $\ell_D, \ell_\Omega \to 0$. The gradient and classical solutions coincide far from the dislocation line and the interface. It is worth noting that all these features are also characteristic for the earlier gradient solutions of dislocation-interface problems [17–19,23].

Another important advantage of the gradient solution is that the maximum stress magnitude can be investigated. Some numerical results are shown in Figures 3 and 4. For a purely elastic interface ($\mu_\Omega \neq \mu_D$ and $\ell_\Omega = \ell_D$), if the nanowire is elastically softer than the matrix ($\mu_\Omega < \mu_D$), the maximum magnitude of the σ_{zy} component, $\max|\sigma_{zy}|$, increases when the dislocation is shifted to the interface (here $\xi \to 20\ell_\Omega$), and the peak of $\max|\sigma_{zy}|$ is achieved when the dislocation reaches the interface (Fig. 3a). In the opposite case (the nanowire is harder than the matrix, $\mu_\Omega > \mu_D$), the value of

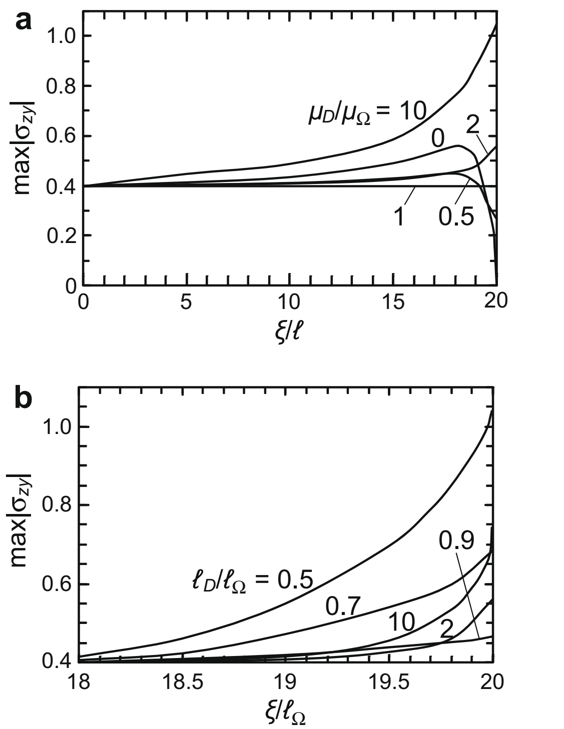

Figure 3. Dependence of the maximum stress magnitude $\max|\sigma_{zy}|$ on the normalized dislocation position ξ/ℓ_Ω in an embedded nanowire of radius $R = 20\ell_\Omega$ (a) for $\ell_\Omega = \ell_D$ and different values of ratio μ_D/μ_Ω, and (b) for $\mu_\Omega = \mu_D$ and different values of ratio ℓ_D/ℓ_Ω. The stress values are given in units of $\mu_\Omega b/(2\pi\ell_\Omega)$.

$\max|\sigma_{zy}|$ first increases, reaches a peak and decreases rapidly when the dislocation comes nearer than $\approx 2\ell$ to the boundary. If the shear moduli are equal ($\mu_\Omega = \mu_D$) but the gradient coefficients are not ($\ell_\Omega \neq \ell_D$), the maximum stress magnitude increases when the dislocation comes close to the interface (Fig. 3b). The peak of $\max|\sigma_{zy}|$ grows when the ratio ℓ_D/ℓ_Ω becomes larger or smaller than 1.

The effect of the nanowire radius R on the maximum stress magnitude $\max|\sigma_{zy}|$ (size effect) in the case of a purely elastic interface is illustrated in Figure 4. For a fixed dislocation position ξ, when $\mu_D > \mu_\Omega$, the smaller nanowire causes a larger $\max|\sigma_{zy}|$, the value of which increases with the ratio of shear moduli μ_D/μ_Ω (Fig. 4a). If $\mu_D < \mu_\Omega$, the peak value of $\max|\sigma_{zy}|$ increases with the nanowire radius (see dashed curves in Fig. 4b) and approaches a horizontal asymptote. In this case, the peak value of $\max|\sigma_{zy}|$ decreases when the ratio μ_D/μ_Ω increases. When $\mu_D = 0$, the behavior of $\max|\sigma_{zy}|$ is very similar to the maximum magnitude of dislocation strain $\varepsilon_{zy}^{(\max)}$ that we studied in our previous paper [22]; it attains zero when the dislocation is situated on the boundary.

In summary, the strain-gradient theory of elasticity gives a smooth and nonsingular solution for the stress field of a screw dislocation inside an embedded nanowire. The maximum magnitude of dislocation stress depends greatly on the dislocation position, the nanowire size and the ratios of the shear moduli of the matrix and nanowire materials. When dislocation occurs near the interface, the maximum magnitude of its stress also

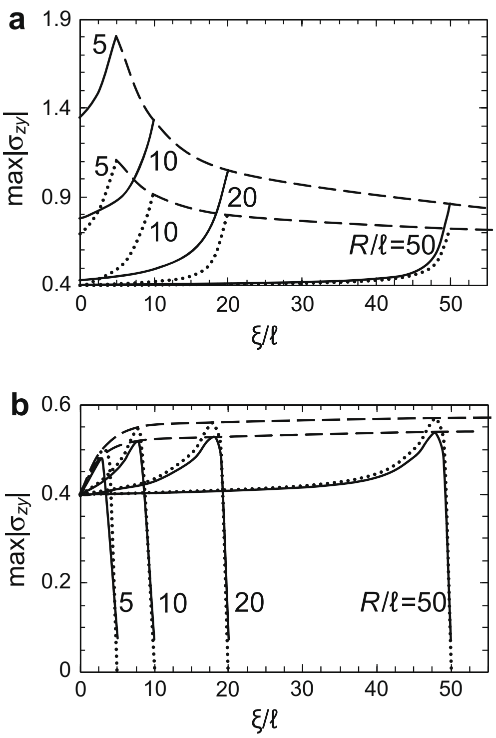

Figure 4. Dependence of the maximum stress magnitude max $|\sigma_{zy}|$ on the normalized dislocation position ξ/ℓ_Ω in an embedded nanowire of normalized radius $R/\ell_\Omega = 5$, 10, 20, and 50 for $\ell_\Omega = \ell_D$ and different values of ratio μ_D/μ_Ω: (a) 5 and 10, and (b) 0 and 0.1. Solid curves correspond to $\mu_D/\mu_\Omega = 0.1$ and 10, dotted curves to $\mu_D/\mu_\Omega = 0$ and 5. Dashed curves show the effect of nanowire radius on the peak value of max $|\sigma_{zy}|$. The stress values are given in units of $\mu_\Omega b/(2\pi\ell_\Omega)$.

varies greatly with the ratio of gradient coefficients. In the case of elastically softer nanowire, the maximum stress magnitude is larger for the dislocation placed in thinner and softer nanowire, closer to the interface. In the opposite case of elastically harder nanowire, the peak value of the maximum stress magnitude is larger for the dislocation placed in thicker and harder nanowire, at a small distance (about ℓ_Ω) from the interface.

K.M.D. and H.M.S. were supported by Sharif University of Technology. M.Yu.G. appreciates the support of the Russian Foundation of Basic Research (Grant 08-02-00304-a).

[1] I.A. Ovid'ko, A.G. Sheinerman, Adv. Phys. 55 (2006) 627.
[2] R. Maranganti, P. Sharma, J. Comput. Theor. Nanosci. 4 (2007) 715.
[3] D. Raabe, Computational Materials Science: The Simulation of Materials, Microstructures and Properties, Wiley-VCH, Weinheim, 1998.
[4] A.N. Cleland, Foundations of Nanomechanics: From Solid-State Theory to Device Applications, Springer, Berlin, 2003.
[5] C.Q. Ru, E.C. Aifantis, MTU Report, Houghton, MI, preprint, 1993.
[6] C.Q. Ru, E.C. Aifantis, Acta Mech. 101 (1993) 59.
[7] A.C. Eringen, J. Appl. Phys. 54 (1983) 4703.
[8] A.C. Eringen, Nonlocal Continuum Field Theories, Springer-Verlag, New York, 2002.
[9] B.S. Altan, E.C. Aifantis, Scripta Metall. Mater. 26 (1992) 319.
[10] R. Maranganti, P. Sharma, J. Mech. Phys. Solids 55 (2007) 1823.
[11] J. Kioseoglou, G.P. Dimitrakopulos, Ph. Komninou, Th. Karakostas, I. Konstantopoulos, M. Avlonitis, E.C. Aifantis, Phys. Status Solidi (a) 203 (2006) 2161.
[12] H.M. Shodja, A. Tehranchi, submitted for publication.
[13] J. Kioseoglou, G.P. Dimitrakopulos, Ph. Komninou, Th. Karakostas, E.C. Aifantis, J. Phys. D: Appl. Phys. 41 (2008) 035408.
[14] M.Yu. Gutkin, E.C. Aifantis, Scripta Mater. 35 (1996) 1353.
[15] M.Yu. Gutkin, E.C. Aifantis, Scripta Mater. 36 (1997) 129.
[16] M.Yu. Gutkin, E.C. Aifantis, Scripta Mater. 40 (1999) 559.
[17] M.Yu. Gutkin, K.N. Mikaelyan, E.C. Aifantis, Scripta Mater. 43 (2000) 477.
[18] M.Yu. Gutkin, K.N. Mikaelyan, E.C. Aifantis, Phys. Solid State 42 (2000) 1652.
[19] K.N. Mikaelyan, M.Yu. Gutkin, E.C. Aifantis, Phys. Solid State 42 (2000) 1659.
[20] M. Lazar, G.A. Maugin, Int. J. Eng. Sci. 43 (2005) 1157.
[21] M. Lazar, G.A. Maugin, Proc. Roy. Soc. A 462 (2006) 3465.
[22] H.M. Shodja, K.M. Davoudi, M.Yu. Gutkin, Scripta Mater. 59 (2008) 368.
[23] K.M. Davoudi, M.Yu. Gutkin, H.M. Shodja, submitted for publication.
[24] M.Yu. Gutkin, E.C. Aifantis, Phys. Status Solidi (b) 214 (1999) 245.
[25] M.Yu. Gutkin, E.C. Aifantis, Phys. Solid State 41 (1999) 1980.
[26] D.J. Unger, E.C. Aifantis, Theor. Appl. Fract. Mech. 34 (2000) 243.
[27] D.J. Unger, E.C. Aifantis, Theor. Appl. Fract. Mech. 34 (2000) 253.
[28] L. Teneketzis Tenek, E.C. Aifantis, Compos. Struct. 53 (2001) 189.
[29] M.Yu. Gutkin, Rev. Adv. Mater. Sci. 13 (2006) 125.
[30] M. Lazar, G. Maugin, Mech. Res. Commun. 33 (2006) 674.
[31] M.Yu. Gutkin, Rev. Adv. Mater. Sci. 1 (2000) 27.
[32] E.C. Aifantis, Mech. Mater. 35 (2003) 259.
[33] J. Dundurs, in: T. Mura (Ed.), Mathematical Theory of Dislocations, A.S.M.E., New York, 1969, pp. 70–115.
[34] K.M. Davoudi, M.Yu. Gutkin, H.M. Shodja, submitted for publication.