Rev.Adv.Mater.Sci. 13 (2006) 77-84

# EMISSION OF GRAIN BOUNDARY DISLOCATIONS BY NANOVOIDS IN DEFORMED POLYSILICON MATERIALS

**S.V. Bobylev, N.F. Morozov and I.A. Ovid'ko**

Institute of Problems of Mechanical Engineering, Russian Academy of Sciences,
Bolshoj 61, Vas.Ostrov, St.Petersburg 199178, Russia

*Received: June 14, 2006*

**Abstract.** A theoretical model is suggested which describes a special mechanism for emission of grain boundary (GB) dislocations by nanovoids (nanoscale voids) in plastically deformed polysilicon materials. In the framework of the model, GB dislocations are emitted from nanovoids by ideal nanoscale shear events under the shear stress action. The characteristic values of the flow stress needed to initiate GB dislocation emission from nanovoids are estimated and shown to be close to those that characterize plastic flow in polysilicon. With the results of the suggested theoretical model, evolution of nanovoids along GBs in polysilicon materials at quasistatic and fatigue load regimes is discussed.

## 1. INTRODUCTION

Polysilicon serves as the dominant constitutional material for integrated circuits and microelectromechanical systems (MEMS) and thereby represents the subject of intensive research; see, e.g., [1-12]. Of crucial importance for performance of MEMS based on polysilicon are its mechanical properties. Commonly, polysilicon shows a brittle behavior at low temperatures, because of high values of the Peierls barrier for lattice dislocation movement [7,9,10]. At the same time, in recent years, delayed fracture of fatigued polysilicon under applied cyclic stresses has been well documented; see, e.g., [5,6,10]. This phenomenon means that damage accumulation and/or plastic deformation precede the complete fracture of polysilicon. Following the results of recent experiments [10], lattice dislocation slip is not significant in polysilicon at low temperatures, while GB sliding – plastic shear along GBs - plays a crucial role in the plastic deformation of polysilicon at low temperatures. Besides GBs, nanovoids often exist in as-fabricated polysilicon for MEMS applications [12]. Also, nanovoids can be intensively nucleated at local stress concentrators in polysilicon during plastic deformation, as with other crystalline materials. In these circumstances, nucleation and evolution of nanovoids under applied stresses can be attributed to damage accumulation in polysilicon. Since nanovoids are typical elements of the defect structure of polysilicon under mechanical load [12], they are expected to strongly affect GB sliding in polysilicon at low temperatures. In particular, nanovoids located at GBs and their triple junctions [12] can serve as effective sources of GB dislocations, carriers of GB sliding. The standard mechanism for emission of GB and lattice dislocations by nanovoids is realized through nucleation of these dislocations at the nanovoid free surface and their further movement into the material surrounding the nanovoid [13,14]. However, the standard mechanism is specified by a rather large energy barrier [13,14] and thereby can provide emission of GB and lattice dislocations by nanovoids in only crystalline materials under shock loading with extremely high applied

---

Corresponding author: I.A. Ovid'ko, e-mail: ovidko@def.ipme.ru

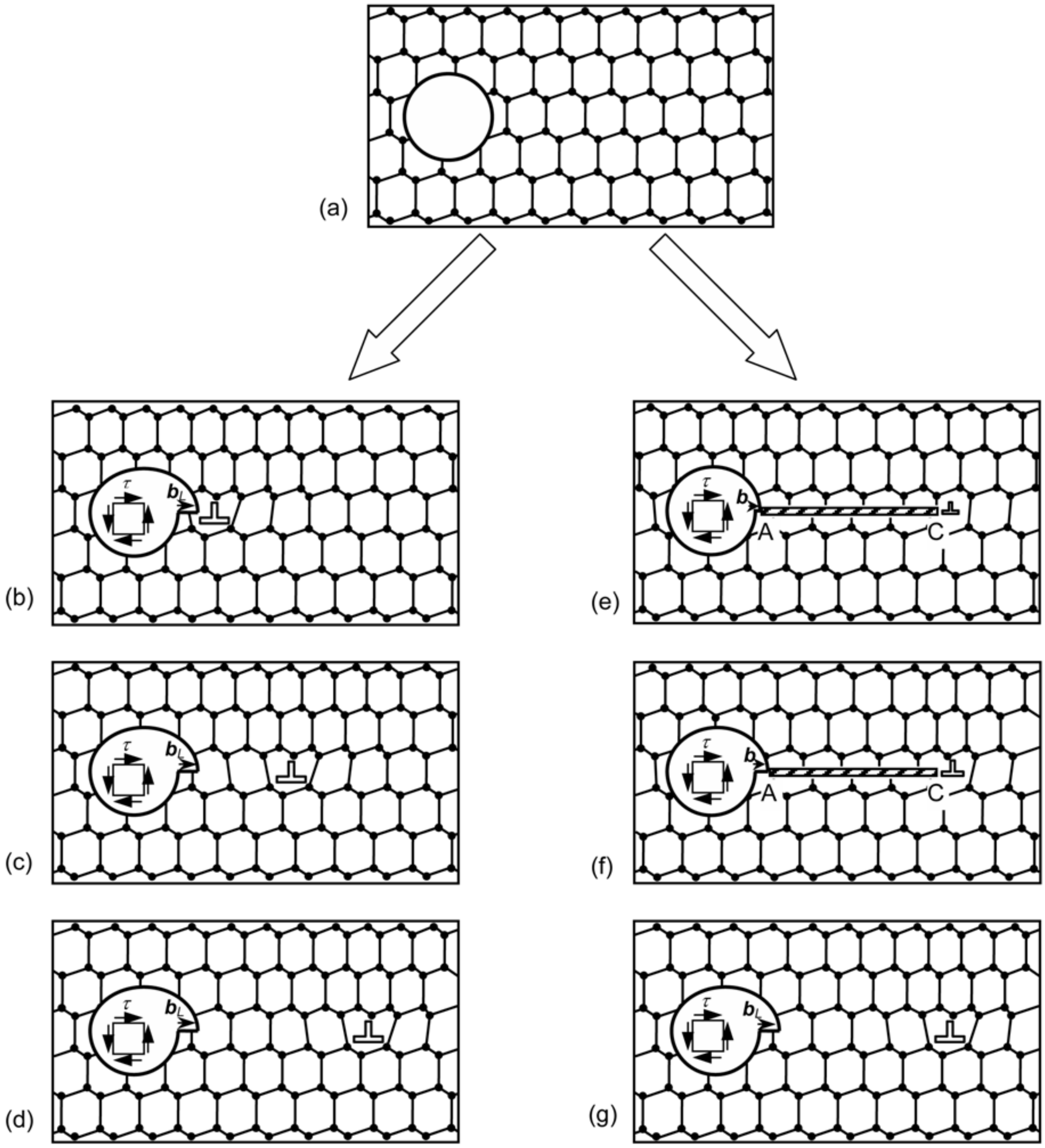

**Fig. 1.** Mechanisms for emission of lattice dislocations in polysilicon (two-dimensional schematic representation). (a) Initial state of silicon containing a nanovoid. (b)-(d) Standard emission mechanism is realized by (b) generation of lattice dislocation at nanovoid free surface and (c, d) its further glide in crystal lattice of silicon. (e)-(g) New emission mechanism involves a nanoscale ideal shear. (e) A nanoscale ideal shear occurs along plane fragment AC and results in the formation of both non-crystallographic partial dislocation with infinitesimal magnitude $s$ of Burgers vector and generalized stacking fault AC. (f) The Burgers vector magnitude $b$ continuously increases and (g) reaches the magnitude $b_L$ that characterizes a perfect lattice dislocation.

stresses [13]. The main aim of this paper is to suggest and theoretically describe a new mechanism for emission of GB dislocations by nanovoids. This mechanism involves a nanoscale ideal shear and is characterized by the absence of any energy barrier for emission of GB dislocations by nanovoids in wide ranges of parameters of polysilicon deformed at low temperatures and comparatively low applied stresses. Also we will discuss the effects of GB dislocation emission from nanovoids on their evolution in polysilicon at quasistatic and fatigue load regimes.

## 2. EMISSION OF DISLOCATIONS FROM NANOVOIDS IN POLYSILICON: STANDARD AND NEW MECHANISMS

Let us discuss the specific features of the standard and new mechanisms for dislocation emission from nanovoids in the exemplary case of lattice dislocations in polysilicon. This case clearly illustrates the difference in geometry between the standard and new mechanisms. Then we will discuss the specific features of emission of GB dislocations from nanovoids in polysilicon.

Let us consider a nanovoid in a polysilicon specimen under mechanical load (Fig. 1a). Figs. 1a–1d show schematically the standard mechanism for dislocation emission from nanovoid. At the beginning of the standard mechanism action, a lattice dislocation nucleates at the nanovoid free surface (Fig. 1b). Then the dislocation glides under the shear stress action from the nanovoid to a surrounding material (Figs. 1c and 1d). During the standard dislocation nucleation and glide processes (Figs. 1a–1d), its Burgers vector magnitude $b_L$ is always constant [13,14]. The calculations [13,14] have shown that the standard mechanism is specified by a rather large energy barrier and thereby can not effectively operate in materials at conventional quasistatic load conditions. The standard mechanism can provide emission of GB and lattice dislocations by nanovoids in only crystalline materials under shock load characterized by extremely high values of the applied stress.

However, dislocation emission from nanovoids in polysilicon and other materials may also occur by a new alternative mechanism, namely the nucleation of a 'non-crystallographic' partial dislocation located at a finite distance from the nanoviod free surface and characterized by a Burgers vector magnitude (hereinafter called strength) $b$ growing from zero to the strength $b_L$ of a perfect lattice dislocation (Figs. 1a, 1e–1g). As to details, the new mechanism for dislocation emission from nanovoids (Figs. 1a, 1e–1g) operates as follows. First, a local momentary ideal shear (a rigid-body shear) occurs along the nanoscale plane fragment AC (Fig. 1e). The momentary ideal shear is characterized by a small shear magnitude $b$ and produces a planar stacking fault generalized AC of a finite nanoscopic length (Fig. 1e). The stacking fault ends at a 'non-crystallographic' partial dislocation characterized by a non-quantized Burgers vector $\boldsymbol{b}$ with quite a small magnitude (strength) $b << b_L$ (Fig. 1e). Then, due to the shear stress action, the partial dislocation strength $b$ continuously increases (Fig. 1f). Finally, the dislocation strength $b$ reaches the strength $b_L$ of a perfect dislocation (Fig. 1g), in which case the stacking fault disappears. (In general, the mechanism can stop at the stage shown in Fig. 1f, in which case it produces a partial dislocation.)

The final state of the system (Fig. 1g) with the dislocation emitted by the new mechanism is identical to that (Fig. 1d) of the system with the dislocation emitted by the standard mechanism. Therefore, the difference between the mechanisms can be not identified by conventional 'ex-situ' experiments. At the same time, the new mechanism for dislocation emission operates by nanoscale ideal shear that has its analog effectively operating in Gum Metal, a special titanium alloy with a low resistance to shear in certain crystallographic planes [15,16]. Following [16], plastic flow in Gum Metal is carried by nanodisturbances, nanoscale dipoles of 'non-crystallographic' partial dislocations characterized by continuously growing strength values and nucleated by nanoscale ideal shear events. Also, a similar mechanism for plastic deformation by nanoscale ideal shear events can operate in nanocomposites [17] and nanocrystalline metals [18] (where standard mechanisms for dislocation nucleation in nanoscale grains are suppressed; see, e.g., [19–21]). This allows us to think that the new mechanism for dislocation emission can operate in polysilicon, although its experimental identification is difficult.

In terms of the dislocation theory, the new mechanism for dislocation emission is described as a continuous growth of the strength $b$ of the dislocation located at a nanoscopic distance from the nanovoid. In doing so, the strength $b$ increases from 0 to $b_L$ , the strength (Burgers vector magnitude) of a perfect lattice dislocation.

Following [14], nanovoids can be characterized by non-zero Burgers vectors, because their nucleation often is accompanied by absorption of dislocations. In the situation where a nanovoid is characterized by a non-zero Burgers vector $\boldsymbol{B}$, the new mechanism for dislocation emission is described in terms of the dislocation theory as a continuous 'transfer' of the Burgers vector $\boldsymbol{B}$ or its part from the dislocated nanovoid to the emitted dislocation. The

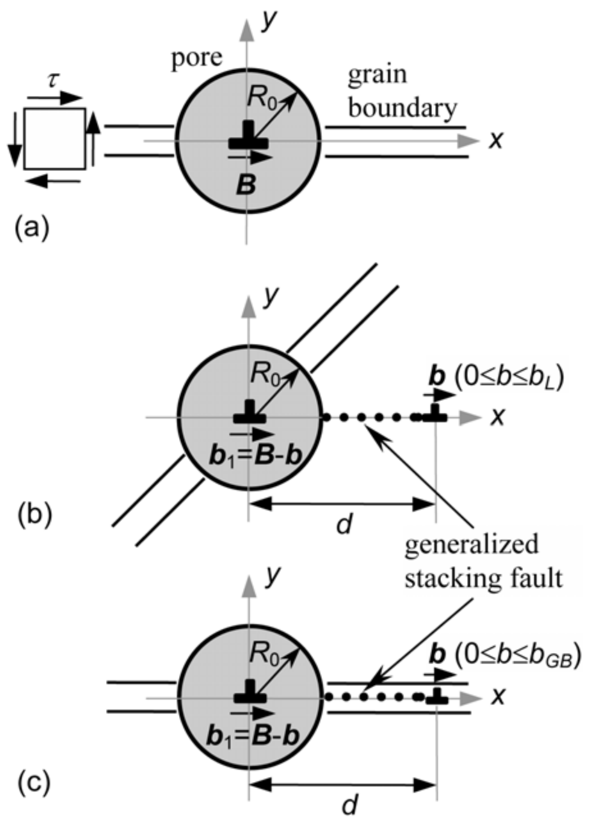

**Fig. 2.** Emission of lattice and grain boundary dislocations from cylindrical nanovoid. (a) Initial state of silicon containing a nanovoid (characterized by Burgers vector ***B***) at grain boundary. (b) Emission of lattice dislocation by nanoscale ideal shear from nanovoid. Lattice dislocation and nanovoid are connected by generalized stacking fault (dotted segment). (c) Emission of grain boundary dislocation by nanoscale ideal shear from nanovoid. Grain boundary dislocation and nanovoid are connected by generalized stacking fault (dotted segment).

dislocation in question is located at a nanoscopic distance from the nanovoid. The continuous growth of the strength *b* of the emitted dislocation is accompanied by a continuous change of the energy of the generalized stacking fault formed between the dislocation and the nanovoid. The change obeys a law that will be discussed in the next section.

Now let us consider the new mechanism for emission of GB dislocations from nanovoids in polysilicon. Perfect GB dislocations serve as carriers of GB sliding [19,22] that serves as the dominant deformation mode in polysilicon at low temperatures [10]. Perfect GB dislocations in a GB are characterized by Burgers vectors being lattice vectors of the dense-shift-complete lattice that describes the GB symmetry [22]. Typical values of the GB Burgers vector magnitude $b_{GB}$ characterizing a perfect GB dislocation are around 0.06-0.10 nm [22].

Emission of a perfect GB dislocation by the new mechanism occurs through a nanoscale ideal shear in the way similar to that shown in Figs. 1e–1g. The main difference between emission events for lattice and GB dislocations (Fig. 2) is in their Burgers vector magnitude. During the emission by a nanoscale ideal shear, a GB dislocation nucleates at a finite distance from the nanovoid, and its characteristic Burgers vector magnitude *b* continuously grows from 0 to $b_{GB}$. The non-perfect GB dislocation and the nanovoid are connected by a generalized stacking fault in the GB plane (Fig. 2c). The stacking fault is not well defined in the GB phase whose structure is more disordered than the perfect crystal structure [18,22]. In any event, the energy density (per unit area) of the generalized stacking fault in an initially disordered GB structure is much lower than that of the ‘true’ stacking fault in a perfect crystal. In this case, the generalized stacking fault formation (Figs. 1e–1h) just slightly influences the GB structure and thereby energy characteristics.

## 3. ENERGY CHARACTERISTICS OF DISLOCATION EMISSION FROM NANOVOIDS IN POLYSILICON

Let us calculate the energy characteristics of the new mechanism for dislocation emission and compare them with those of the standard mechanism. To do so, consider a model dislocated nanovoid in a deformed polysilicon subjected to the action of an external shear stress $\tau = \tau_{xy}$ (Fig. 2). Such a nanovoid can serve as a dislocation source as schematically shown in Fig. 2. For simplicity of mathematics, the nanovoid is assumed to have a cylindrical form (Fig. 2). Also, we suppose that the nanovoid has a radius $R_0$ and is characterized by a Burgers vector ***B*** (Fig. 2a). Emission of dislocations from a dislocated nanovoid - nanovoid characterized by a non-zero Burgers vector ***B*** - is evidently enhanced compared to that from a non-dislocated nanovoid. It is due to the effects of the stresses created by the dislocated nanovoid.

Figs. 2b and 2c illustrate the dislocation emission processes by the new mechanism for lattice and GB dislocations, respectively. The generalized stacking fault of length *d* is shown as dashed segment. To calculate the energy characteristics of the emission processes, we will use formula for the energy change $\Delta W'$ of the system due to nucleation of a dislocation characterized by Burgers vector $\boldsymbol{b}$ and located at a distance $d$ from the nanovoid. This formula is as follows [14]:

$$\Delta W' = \frac{Db^2}{2}\left\{\ln\frac{R_0}{r_0} + \ln\left(\tilde{d}^2 - 1\right)\right\} + \frac{Db^2}{2}\left\{1 - \frac{B}{b}\left(2\ln\tilde{d} - \frac{1}{\tilde{d}^2}\right)\right\} - \frac{Db^2}{2}\left\{\frac{2\tau R_0}{Db}\left(\tilde{d} - \frac{2}{\tilde{d}} + \frac{2}{\tilde{d}^3}\right)\right\}. \qquad (1)$$

Here $D = G/[2\pi(1-\nu)]$, $\tilde{d} = d/R_0$, $G$ denotes the shear modulus, $\nu$ the Poisson ratio, $R_0$ the nanovoid radius, and $r_0$ the screening length for the stress field of the dislocation with strength $b$.

In an analysis of the dislocation emission by a nanoscale ideal shear (Fig. 2), besides the energy change given by formula (1), the energy of the generalized stacking fault should be taken into account. In the case of GB dislocation emission by a nanoscale ideal shear (Fig. 2c), following the approach [18], the energy $W_\gamma^{GB}$ of the generalized stacking fault is approximated by a periodic function of $b$ in the range from 0 to $b_{GB}$, and the result reads:

$$W_\gamma^{GB} = \lambda\gamma_0 d \sin\frac{\pi b}{b_{GB}}, \qquad (2)$$

where $\gamma_0$ is the specific energy density (per unit area) of the standard stacking fault in crystalline silicon (bulk phase), $\lambda$ is the factor taking into account the effect of a disorder of GB structures on the generalized stacking fault energy in a GB ($\lambda < 1$; see a discussion in the end of section 2), and $b_{GB}$ is the Burgers vector magnitude $b_{GB}$ characterizing a perfect GB dislocation. In the framework of the model suggested, the energy $W_\gamma^{GB}$ of the generalized stacking fault is approximated by a periodic function of $b$ in the range from 0 to $b_{GB}$, in which case it reaches its maximum value of $W_\gamma^{GB} = \lambda\gamma_0 d$ at $b = b_{GB}/2$ and is equal to 0 ($W_\gamma^{GB} = 0$) at $b = b_{GB}$. Finally, the emission of GB dislocations from nanovoids (Fig. 2 c) in deformed polysilicon is characterized by the energy change

$$\Delta W_{GB} = \Delta W' + W_\gamma^{GB}, \qquad (3)$$

where $\Delta W'$ and $W_\gamma^{GB}$ are given by formulas (1) and (2), respectively.

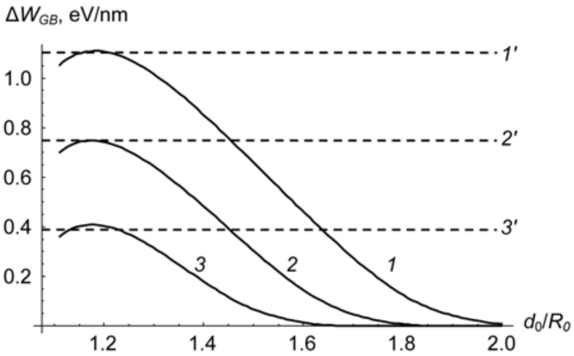

**Fig. 3.** Dependence of the energy barrier (that hampers emission of grain boundary dislocation) on ratio of the distance $d_0$ (between the dislocation and nanovoid in silicon) to nanovoid radius $R_0$. Calculations are performed for emission from a nanovoid of radius $R_0=10b_L$ under the action of external shear stress $\tau$ = 1 GPa. Curves *1*, *2* and *3* correspond to nanovoid Burgers vector magnitudes $B$=0, 0.25$b_L$, 0.5$b_L$, respectively. Dashed curves *1'*, *2'* and *3'* show the corresponding values of the energy barrier for GB dislocation emission by the standard mechanism.

In the situation with emission of lattice dislocations, one can use results of several computer simulations [23–25] of the energy of the generalized stacking fault in silicon. The calculated values of the energy vary widely depending on the calculation technique. However, for even the lowest level of the energy, our corresponding estimates show the lattice dislocation emission by nanovoids (Fig. 2 b) to be energetically unfavorable at realistic values of the applied stress. In these circumstances, we will focus our further consideration on the situation with emission of GB dislocations in deformed polysilicon.

Formulas (1)-(3) allow us to calculate the dependence of the energy barrier (that hampers emission of GB dislocation) on the distance $d_0$ between the dislocation and nanovoid in polysilicon. In doing so, we use the following typical values of parameters for silicon [24]: $G$ = 63.75 GPa, $\nu$ = 0.26, $\gamma_0$= 0.06 J/m², and the lattice parameter $a$ = 0.543 nm. Typical magnitude of Burgers vector characterizing a perfect lattice dislocation in silicon is $b_L = a/\sqrt{2}$, while magnitude of Burgers vector characterizing a GB dislocation is supposed to be $b_{GB}$ = 0.1 nm. Also, the screening length for the dislocation stress field and the factor $\lambda$ are taken as

$r_0 = b$ and $\lambda \approx 0.1$ [18], respectively. Fig. 3 presents results of our calculations of the energy barrier for GB dislocation emission by nanoscale ideal shear events (Fig. 2 c) from a nanovoid of radius $R_0 = 10b_L$, for various values of the Burgers vector magnitude $B$ characterizing the nanovoid under the action of external shear stress $\tau = 1$ GPa. The dependences (Fig. 3) of the energy barrier on the distance $d_0$ between the dislocation and nanovoid in polysilicon are calculated by formulas (1)–(3). Dashed lines in Fig. 3 show the corresponding values of the energy barrier for GB dislocation emission by the standard mechanism. These values (Fig. 3) are calculated by formula (1) of paper [14]. From Fig. 3 it follows that the energy barrier for GB dislocation emission by nanoscale ideal shear events decreases with rising the distance $d_0$ (between the dislocation and nanovoid) and even becomes 0 at critical distance $d_{bl}$. That is, the GB dislocation emission by nanoscale ideal shear events can occur as a non-barrier process in certain ranges of parameters of the system under consideration.

The dependence of the critical distance $d_{bl}$ (at which the transition from barrier to non-barrier GB dislocation emission occurs) on the applied stress is presented in Fig. 4. In calculation of this dependence, the same values of parameters have been used as with calculation of the energy barrier in Fig. 3. From Fig. 4 it follows that the critical distance decreases with rising the applied stress level. That is, the GB dislocation emission by nanoscale ideal shear events enhances when the applied stress increases. Also, note that, following our theoretical analysis, the GB dislocation emission by the new mechanism occurs in the non-barrier way in polysilicon at values of the applied stress < 2GPa (Fig.4). The stress level < 2GPa is smaller than experimentally measured values of the strength (around 2.7 GPa) of polysilicon in the standard monotonic bend test, a version of quasistatic loading [10]. Consequently, the GB dislocation emission by the new mechanism can effectively occur in polysilicon deformed at realistic values of the applied stress.

## 4. EVOLUTION OF NANOVOIDS AT GRAIN BOUNDARIES IN POLYSILICON AT QUASISTATIC AND FATIGUE LOAD REGIMES

Let us discuss the specific features of evolution of nanovoids at grain boundaries in polysilicon at quasistatic and fatigue load regimes. With the results of our theoretical analysis given in the previous sections, nanovoids can effectively emit GB dislocations in polysilicon quasistatically deformed at realistic values of the applied stress <2GPa. In these circumstances, numerous events of GB dislocation emission can induce irreversible elongation of nanovoids as shown in Fig. 5.

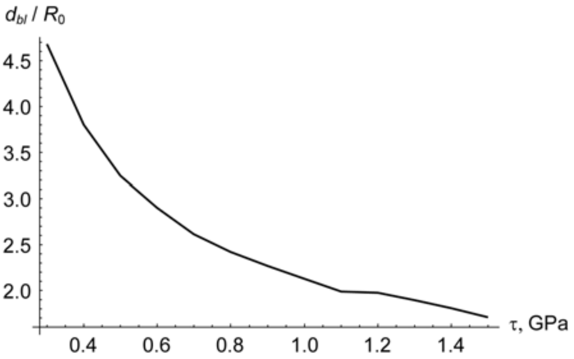

**Fig. 4.** Dependence of critical distance $d_{bl}$ (at which the transition from barrier to non-barrier grain boundary dislocation emission occurs) on the applied stress, for nanovoid radius $R_0 = 10b_L$ and nanovoid Burgers vector magnitude $B$=0.

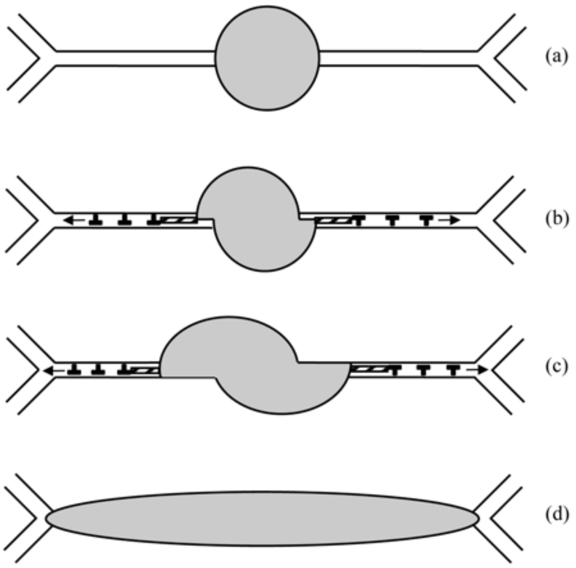

**Fig. 5.** Elongation of nanovoid due to numerous events of emission of grain boundary dislocations by the new mechanism in deformed polysilicon.

In the case of fatigue load of polysilicon, GB dislocation emission and associated evolution of nanovoids have their specific features differing them from those occurring in polysilicon under a quasistatic load. In general, fatigue cycling is characterized by the load ratio *F* defined as the ratio of the minimum stress to the maximum stress in the cycle. A tensile stress is taken as positive, while a compressive stress is taken as negative. The commonly used fatigue load tests are symmetric tension/compression stress cycling (*F* = –1), non-symmetric tension/compression stress cycling (0 > *F* > –1) and zero/tension stress cycling (*F* = 0). In the typical second and third cases (*F* = 0 and 0 > *F* > –1, respectively), during one cycle, the applied stress causes GB dislocation emission and associated evolution of nanovoids to occur in the way similar to that in polysilicon under a quasistatic mechanical load. In the first approximation, one expects that in consideration of the effect of cyclic loading on these processes, one can replace the cyclic stress by the mean applied stress over the cycle.

For symmetric tension/compression stress cycling (*F* = –1), during one cycle, any events of GB dislocation emission and associated evolution of nanovoids occurring due to the action of an applied tensile stress is compensated by that due to the action of an applied compressive stress. Therefore, tension/compression stress cycling hardly can cause the irreversible evolution of nanovoids, shown in Fig. 5. However, the irreversible evolution may occur in response to additional stresses induced by stress concentrators. For instance, polysilicon parts of MEMS often have non-flat free surfaces with notches and other geometric irregularities playing the role of stress concentrators. These stress concentrators provide both additional stresses acting in GB planes and thereby the irreversible evolution of nanovoids (Fig. 5). In this situation, in an analysis of nanocrack formation, one should operate with the effects of the local mean stress near a stress concentrator in the cycle.

## 5. CONCLUDING REMARKS

Thus, in this paper a new mechanism for emission of GB dislocations by nanovoids in deformed polysilicon has been suggested. The mechanism represents the nucleation of 'non-perfect' GB dislocation located at a finite distance from nanovoid and characterized by continuously growing Burgers vector magnitude (Fig. 2c). According to our analysis of the energy characteristics of this mechanism, it can effectively operate in a non-barrier regime in deformed polysilicon. Nanovoids can effectively grow (elongate) along GBs by emission of GB dislocations in deformed polysilicon at quasistatic and non-symmetric cyclic load regimes. Curved free surfaces serve as stress concentrators capable of initiating both the emission of GB dislocations from nanovoids and their elongation in polysilicon specimens under symmetric tension/compression cyclic load.

## ACKNOWLEDGEMENTS

The work was supported by the Sandia National Laboratories (Contract No. 499338), the Aristotle University of Thessaloniki (Subcontract of the Contract HPRN-CT-2002-00198), Russian Academy of Sciences Program 'Structural Mechanics of Materials and Construction Elements', Federal Agency of Science and Innovations (grant of the President of the Russian Federation MK-2902.2005.1).

## REFERENCES

[1] M. Esashi and T. Ono // *J. Phys. D: Appl. Phys.* **38** (2005) R223.
[2] C.L. Muhlstein, R.T. Howe and R.O. Ritchie // *Mech. Mater.* **36** (2004) 13.
[3] H. Kahn, A.Q. He and A.H. Heuer // *Phil. Mag. A* **82** (2002) 137.
[4] K. Gall, M.L. Dunn, Y. Zhang and B.A. Corff // *Mech. Mater.* **36** (2004) 45.
[5] H. Kahn, R. Ballarini, J.J. Bellante and A.H. Heuer // *Science* **298** (2002) 1215.
[6] D.H. Aslem, E.A. Stach and R.O. Ritchie // *Appl. Phys. Lett.* **86** (2005) 041914.
[7] C.L. Muhlstein, E.A. Stach and R.O. Ritchie // *Acta Mater.* **50** (2002) 3579.
[8] C.L. Muhlstein and R.O. Ritchie // *Int. J. Fracture* **119**/**120** (2003) 449.
[9] H. Kahn, R. Ballarini and A.H. Heuer // *Current Opinion Solid State Mater. Sci.* **8** (2004) 71.
[10] H. Kahn, L. Chen, R. Ballarini and A.H. Heuer // *Acta Mater.* **54** (2006) 667.
[11] R.F. Cook // *J. Mater. Sci.* **41** (2006) 841.
[12] P. Shrotriya, S.M. Allameh and W.O. Soboyejo // *Mech. Mater.* **36** (2004) 35.
[13] V.A. Lubarda, M.S. Schneider, D.H. Kalantar, B.A. Remington and M.A. Meyers // *Acta Mater.* **52** (2004) 1397.
[14] I.A. Ovid'ko and A.G. Sheinerman // *Rev. Adv. Mater. Sci.* **11** (2006) 46.
[15] T. Saito, T. Furuta, J.-H. Hwang, S. Kuramoto, K. Nishino, N. Suzuki, R. Chen, A. Yamada, K. Ito, Y. Seno, T. Nonaka, H. Ikehata, N. Nagasako, C. Iwamoto, Y. Ikuhara and T. Sakuma // *Science* **300** (2003) 464.
[16] M.Yu. Gutkin, T. Ishizaki, S. Kuramoto and I.A. Ovid'ko // *Acta Mater.* **54** (2006) 2489.

[17] I.A. Ovid’ko and A.G. Sheinerman // *J. Phys.: Condens. Matter* **18** (2006) L225.

[18] M.Yu. Gutkin and I.A. Ovid’ko // *Appl. Phys. Lett.* **88** (2006) 211901.

[19] M.Yu. Gutkin and I.A. Ovid’ko, *Plastic Deformation in Nanocrystalline Materials* (Berlin, Heidelberg, New York: Springer, 2004).

[20] D. Wolf, V. Yamakov, S.R. Phillpot, A.K. Mukherjee and H. Gleiter // *Acta Mater.* **53** (2005) 1.

[21] B.Q. Han, E. Lavernia and F.A. Mohamed // *Rev. Adv. Mater. Sci.* **9** (2005) 1.

[22] A.P. Sutton and R. W. Balluffi, *Interfaces in Crystalline Materials* (Oxford Science Publications, Oxford, 1996).

[23] E. Kaxiras and M.S. Duesbery // *Phys. Rev. Lett* **70** (1993) 3752.

[24] B. Joós, Q. Ren, M.S. Duesberry // *Phys. Rev. B* **50** (1994) 5890.

[25] M. Miyata and T. Fujiwara // *Phys. Rev. B* **63** (2001) 045206.