

# CRITICAL STRESS FOR DISLOCATION FORMATION IN DEFORMED TWINNED NANOWIRES

S.V. Bobylev<sup>1,2,3</sup> and A.G. Sheinerman<sup>1,2,3</sup>

<sup>1</sup>Department of Mathematics and Mechanics, St. Petersburg State University, St. Petersburg 198504, Russia

<sup>2</sup>Institute of Problems of Mechanical Engineering, Russian Academy of Sciences, St. Petersburg 199178, Russia

<sup>3</sup>Research Laboratory for Mechanics of New Nanomaterials, Peter the Great St. Petersburg Polytechnical University, St. Petersburg 195251, Russia

Received: September 12, 2015

**Abstract.** A model is suggested that describes the generation of dislocations in twinned nanowires under tension. The critical stress for dislocation formation in deformed twinned nanowires is calculated. It is shown that the strong twin size dependence of the critical stress is associated with the nanowire surface effects, such as dislocation attraction by the nanowire surface and the presence of the surface steps and surface stresses. The calculations demonstrate that the dependence of the critical stress on the nanowire twin thickness can be described by a Hall-Petch type relation, in agreement with recent experimental data.

## 1. INTRODUCTION

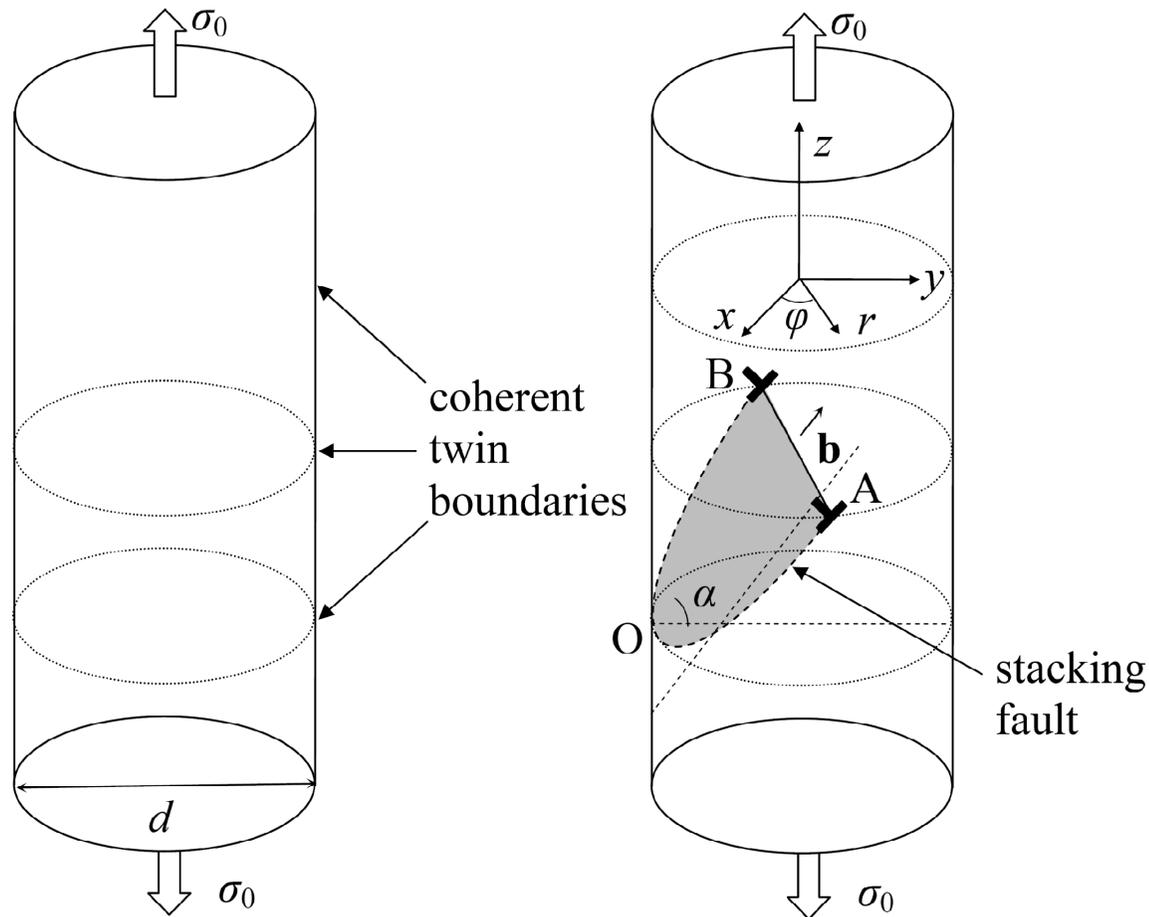
Last years, metal nanowires have drawn much attention as potential structural elements of next-generation electronic devices, from nanotransistors and data storage devices to nanosensors [1–5]. Along with high conductivity, high strength of such nanowires is a crucial property required for their applications. Recently, a new approach for enhancing the strength of metal nanowires has been proposed, which lies in the synthesis of nanowires containing coherent twin boundaries normal to the nanowire axis [6–10]. In particular, experiments [6–10] demonstrated that the presence of a high density of twin boundaries in copper or gold nanowires can lead to a dramatic increase in their strength and, at the same time, provides essential tensile ductility. To elucidate the effects of twins on strength and ductility of twinned nanowires, a number of molecular dynamics simulations have been performed [11–25]. The simulations [11–25] confirmed that the yield strength of twinned nanowires as well

as the critical stress for dislocation nucleation in such nanowires increases, as a rule, with decreasing twin thicknesses, but provided quite different quantitative dependences of the yield stress on twin thickness. For example, Deng and Sansoz [17,18] derived a linear dependence of the yield stress on the inverse of twin thickness. Guo and Xia [20] reported the existence of both hardening and softening behavior of twinned nanowires: in their simulations, the yield strength first decreased and then increased with increasing twin thickness. Hammami and Kulkarni [24] reported that the yield stress first decreases with increasing twin thickness and then (above twin thickness of 2 to 4 nm) becomes independent on twin thickness. Gao et al. [25] revealed three twin thickness intervals where the yield strength is in a linear dependence with the inverse of twin thickness, but with different slopes.

Also, recently, Wang et al. [10], using in situ high-resolution transmission electron microscopy, measured the critical strain for dislocation nucle-

---

Corresponding author: S.V. Bobylev, e-mail: bobylev.s@gmail.com



**Fig. 1.** Model for dislocation generation in a twinned cylindrical nanowire under the action of a uniform tensile load  $\sigma_0$ . (a) Initial defect-free state of the nanowire. (b) Partial edge dislocation AB with the Burgers vector  $\mathbf{b}$  nucleates from the intersection of the surface and a twin boundary and stops at the adjacent twin boundary. The dislocation leaves a stacking fault (shown as a grey region) behind itself.

ation in twinned gold nanowires under tension. They obtained a Hall-Petch type relationship between the critical strain  $\varepsilon_c$  and twin thickness  $h$  that can be written as  $\varepsilon_c = \varepsilon_{c0} + kh^{1/2}$ , where  $\varepsilon_{c0}$  and  $k$  are parameters. As in paper [9], they also revealed that at very small twin thicknesses, twinned gold nanowires demonstrate near-ideal theoretical strength. Besides, they showed that the results of previous molecular dynamics simulations [9,18] can be interpolated by Hall-Petch type dependences down to a twin thickness of 2–3 nm, below which the homogeneous nucleation of dislocation dipoles inside the nanotwinned nanowire becomes an alternative to the heterogeneous dislocation nucleation from the free surface [10].

Thus, both experiments and simulations demonstrate a strong dependence of the yield strength and the critical stress for dislocation nucleation (which can be considered as the lower bound for the yield strength) in twinned nanowires on twin thickness. At the same time, the reason for a dramatic increase in the yield strength due to high-density twins in twinned nanowires is not quite clear. Previous papers [17,20] attributed the twin thickness dependence of the yield strength in twinned nanowires to the anisotropy of nanowires, which creates repulsive forces exerted on dislocations by twin boundaries. At the same time, the analytical

estimates in papers [17,20] did not account for the nanowire surface effects (dislocation attraction to the nanowire free surface, surface steps and surface stresses), which, due to relatively low elastic anisotropy of metallic nanowires, should have much stronger effect on dislocation generation than the elastic interaction of dislocations with twin boundaries. To fill this gap, in the present paper, we suggest a model that describes the generation of dislocations in deformed twinned nanowires with an account for the nanowire surface effects, calculate the critical stress for dislocation formation and compare it with available experimental data.

## 2. DISLOCATION IN A TWINNED NANOWIRE. MODEL

Consider a model [111]-oriented twinned cylindrical nanowire with a face-centered cubic (fcc) crystal lattice under a uniaxial tensile load  $\sigma_0$  whose direction coincides with the nanowire axis (Fig. 1a). We assume that the twin boundaries in the nanowire are normal to the nanowire axis and the thicknesses of all the twins are the same. We denote the nanowire diameter as  $d$  and the twin thickness as  $h$ . Let us examine the generation of a dislocation in the nanowire (Fig. 1b). Based on the results of experiments and computer simulations [10–25], we

assume that the dislocation is the Shockley partial, has the slip system  $(11\bar{1})[112]$  and nucleates from the intersection of a twin boundary with the lateral nanowire surface (labeled as point O in Fig. 1b). The dislocation Burgers vector  $\mathbf{b}$  makes the angle  $\alpha = \arccos(1/3) \approx 70.5^\circ$  with the nanowire cross section, and the Burgers vector magnitude  $b$  is related to the crystal lattice parameter  $a$  by the relation  $b = a/\sqrt{6}$ .

In general, the nucleating dislocation represents a dislocation semiloop whose exact shape can vary. Therefore, for definiteness, we suppose that the dislocation line represents a straight segment whose length increases as the dislocation moves inside the nanowire (Fig. 1b). Then the dislocation has the edge character. Within the model, under the action of the applied load, the dislocation moves from the intersection of the nanowire free surface with a twin boundary towards the adjacent twin boundary, leaving behind a stacking fault (see the grey region in Fig. 1b), which connects the dislocation line with the nanowire surface. Since the twin boundary serves as a barrier for dislocation motion, at the twin boundary the dislocation stops (Fig. 1b).

Unless the applied load is very high, the generated dislocation has to overcome some energetic barrier. Recent experiments and computer simulations [26,27] of dislocation nucleation in single crystal Cu and Ni nanowires demonstrated that thermal fluctuations significantly promote dislocation nucleation in nanowires and can dramatically reduce the critical stress for dislocation nucleation in such nanowires. If the applied load is sufficient for the dislocation to overcome the energetic barrier via thermal fluctuations, the latter can nucleate and move to the nearest twin boundary. However, the generated dislocation should be stable in the course of nanowire deformation and ought to resist its reverse motion to the free surface (driven by dislocation attraction to the free surface and thermal fluctuations). This means that dislocation nucleation within a specified time period should be more likely than its disappearance within the same time period. In turn, this can be realized if the energetic barrier to generate the dislocation and move it to the nearest twin boundary is smaller than that required to move the dislocation back from the twin boundary to the nanowire surface. The latter condition can be presented as  $\Delta W < 0$ , where  $\Delta W$  is the energy variation associated with the dislocation formation at the twin boundary (Fig. 1b). This condition for dislocation formation has been extensively used in consideration of dislocation formation in thin films on planar substrates (see, e.g., book [28]) and two-layer

nanowires [29–34] and nanoparticles [34]. To calculate the critical stress for dislocation formation in a twinned nanowire, in the following section we calculate the energy change  $\Delta W$  associated with dislocation formation at the nanowire twin boundary.

### 3. CRITICAL STRESS FOR DISLOCATION FORMATION IN A TWINNED NANOWIRE

Let us calculate the energy change  $\Delta W$  associated with dislocation formation at the nanowire twin boundary. The energy  $\Delta W$  can be presented as

$$\Delta W = W_d + W_{sf} + W_{step} - A, \quad (1)$$

where  $W_d$  is the proper energy of the dislocation (including the energy of the dislocation core),  $W_{sf}$  is the stacking fault energy,  $W_{step}$  is the energy of the step formed at the nanowire surface due to dislocation generation, and  $A$  is the work of the mechanical stresses (acting in the nanowire in the absence of the dislocation) done on dislocation motion from the nanowire surface to the twin boundary.

Let us calculate the proper energy  $W_d$  of the dislocation in the nanowire (Fig. 1b). Since deriving a rigorous analytical calculation for the proper energy of such a dislocation in the nanowire is extremely complicated, we make a simple estimate of this energy using the approach [35] employed previously for the calculation of the proper dislocation energy in single crystalline nanowire with a square cross section. (This approach is also similar to other techniques used for the approximate calculation of the proper energies of dislocations in nanowires [32,36] and quantum dot [37].) In this approach, the proper strain energy of the dislocation in a nanowire is presented as the sum of the self-energies of small dislocation segments, while the energy of each segment is calculated based on its distance from the nanowire surface. To be more specific, the energy of each dislocation segment (per its unit length) lying at a distance  $R'$  from the nanowire surface is calculated as the energy of an infinite edge dislocation (per its unit length) in a semi-infinite isotropic solid with a flat free surface, situated at the distance  $R'$  from this flat free surface. Thus, the strain energy  $W$  of each dislocation segment (per its unit length) can be presented as  $W = (Db^2/2)\ln(R'/r_0)$ , where  $D = G/[2\pi(1 - \nu)]$ ,  $G$  is the shear modulus,  $\nu$  is Poisson's ratio,  $r_0 \approx b$  is the dislocation core cut-off radius.

Let  $p$  be the distance from the central point of the dislocation line shown in Fig. 1b to the nanowire surface ( $p = h/\tan\alpha$ ). Then the length  $L$  of the dislo-

cation line can be written as  $L = 2\sqrt{p(d-p)}$  (see Fig. 2). For an infinitesimal dislocation segment with a length  $dl$  situated at a distance  $l$  from the dislocation central point (see Fig. 2), its distance  $R'$  to the nanowire surface follows as

$$R' = d/2 - \sqrt{(d/2 - p)^2 + l^2}. \quad (2)$$

The proper strain energy  $dW_d$  of this dislocation segment is as follows:

$$dW_d = (Db^2/2) \ln(R'/b) dl. \quad (3)$$

Integrating the latter expression over the dislocation line, accounting for formula (2) and adding the energy  $W_c = (Db^2/2)L$  [38] of the dislocation core, one obtains

$$W_d = W_c + \frac{Db^2}{2} \int_{-\sqrt{p(d-p)}}^{\sqrt{p(d-p)}} \ln \frac{R'}{b} dl = Db^2 \left[ \frac{d}{2} \ln \frac{|d/2 - p|}{d/2 + \sqrt{p(d-p)}} + \sqrt{p(d-p)} \ln \frac{2p(d-p)}{|d/2 - p|b} \right]. \quad (4)$$

The energy  $W_{sf}$  of the stacking fault is presented in the form

$$W_{sf} = \gamma_{sf} S_{sf}, \quad (5)$$

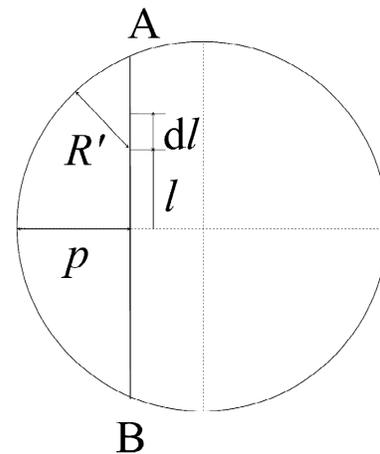
where  $\gamma_{sf}$  is the specific (per unit area) stacking fault energy,  $S_{sf}$  is the area of the stacking fault (see the grey region in Fig. 1b). The area  $S_{sf}$  can be calculated as the area of a segment of the ellipse with the semi-axes  $d/\cos\alpha$  and  $d$  as [39]

$$S_{sf} = \frac{1}{4 \cos \alpha} \times \left( d^2 \arccos \frac{d-2p}{d} - 2(d-2p)\sqrt{p(d-p)} \right). \quad (6)$$

The energy  $W_{step}$  associated with the formation of the surface step is calculated as

$$W_{step} = \beta \gamma S_{step}, \quad (7)$$

where  $\gamma$  is the specific (per unit area) surface energy,  $S_{step}$  is the area of the surface step, and  $\beta$  is the pre-factor ( $\beta < 1$ ) that accounts for the atomic-scale nanowire surface roughness prior to dislocation nucleation. The surface step area  $S_{step}$  can be roughly estimated as the product of the step length  $l_{AOB}$  (equal to the length of the ellipse arc AOB in Fig. 1b) and the dislocation Burgers vector magni-



**Fig. 2.** Nanowire cross section containing dislocation line AB whose position is determined by the parameter  $p$ .

tude  $b$ . Using the known formula [39] for the length of an ellipse arc, one obtains

$$S_{step} \approx b l_{AOB} = \frac{bd}{\cos \alpha} \times [E(\pi/2, \sin \alpha) - E(\arcsin(1 - 2p/d), \sin \alpha)], \quad (8)$$

where  $E(\varphi, k)$  is the elliptic integral of the second kind.

The work  $A$  of the mechanical stresses on dislocation motion is given by

$$A = \tau b S_{sf}, \quad (9)$$

where  $\tau$  is the resolved shear stress acting in the dislocation slip plane in the absence of the dislocation. The shear stress  $\tau$  is created by the applied tensile load  $\sigma_0$  and the internal elastic stresses (associated with the presence of the nanowire surface), which, as known [40,41], can reach high values in the nanowires and nanoparticles with small diameters. To calculate the internal elastic stresses in the bulk of the nanowire, one should note that the nanowire surface gives rise to the surface stresses [40], which are determined by the values of the nanowire surface energy and its derivatives with respect to strains at the surface. In calculating the internal stresses, for simplicity, we neglect the contribution of the surface elastic moduli (relating the surface stresses with the strains at the surface), whose effect is small as long as the nanowire diameter  $d$  does not exceed 4 to 6 nm [41]. (This also allows us to neglect the effect of the surface stresses on the proper energy of the dislocation.) We also assume that the properties of the surface are isotropic, as is the case with the bulk material. Then in the cylindrical coordinate system  $(r, \varphi, z)$  associated with the nanowire (Fig. 1b), the stress field acting in the nanowire in the absence of the dislocation reads [41]

$$\sigma_{rr} = \sigma_{\phi\phi} = -\frac{2f}{d}, \quad \sigma_{zz} = \sigma_0 - \frac{4f}{d}, \quad (10)$$

where  $f = \gamma + \partial\gamma/\varepsilon_{zz}$  and  $\varepsilon_{zz}$  is the elastic strain tensor component at the nanowire surface. From formula (10), we obtain the resolved shear stress  $\tau$  as follows:

$$\tau = (\sigma_{zz} - \sigma_{rr}) \cos \alpha \sin \alpha = \left( \sigma_0 - \frac{2f}{d} \right) \cos \alpha \sin \alpha. \quad (11)$$

From (9) and (11) one obtains

$$A = bS_{sf} \left( \sigma_0 - \frac{2f}{d} \right) \cos \alpha \sin \alpha. \quad (12)$$

Now the total energy change  $\Delta W$  associated with dislocation formation at the twin boundary follows from (1), (4–(8) and (12) as

$$\Delta W = Db^2 \left[ \frac{d}{2} \ln \frac{|d/2 - p|}{d/2 + \sqrt{p(d-p)}} + \sqrt{p(d-p)} \ln \frac{2p(d-p)}{|d/2 - p|b} \right] + \beta\gamma S_{step} + \left[ \gamma_{sf} - b \left( \sigma_0 - \frac{2f}{d} \right) \cos \alpha \sin \alpha \right] S_{sf}. \quad (13)$$

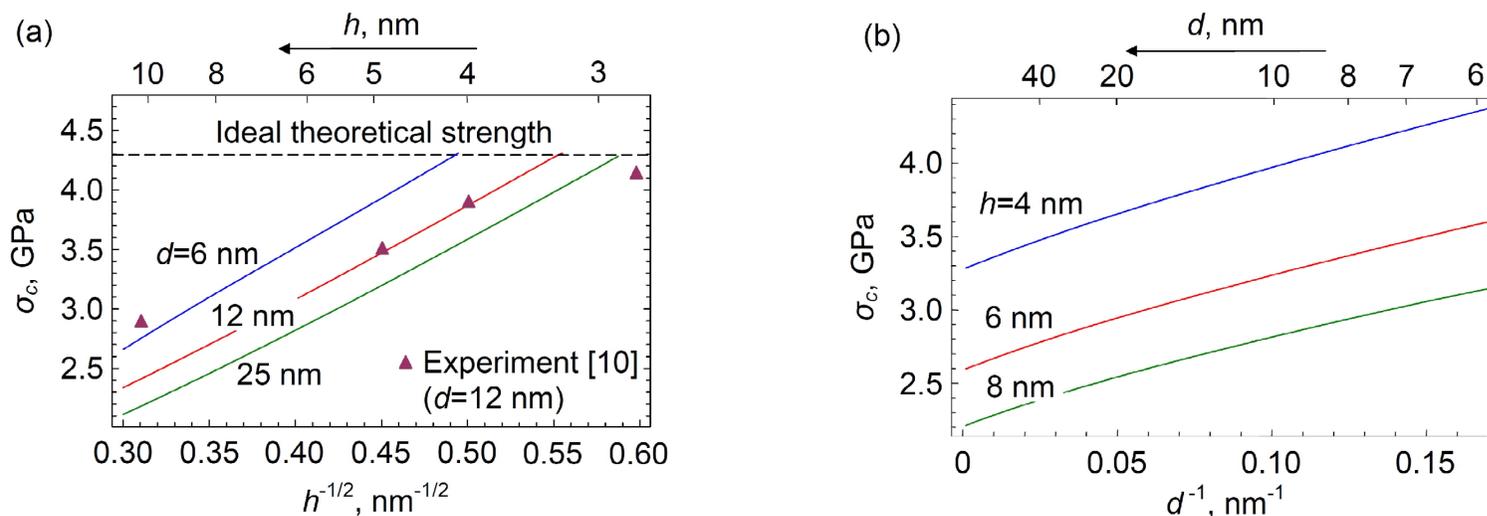
where  $S_{sf}$  and  $S_{step}$  are given by formulae (6) and (8), respectively, and  $p = h/\tan \alpha$ .

Let us estimate the critical stress  $\sigma_c$  for dislocation formation in the nanowire (Fig. 1b). This stress is calculated from the critical condition  $\Delta W|_{\sigma_0 = \sigma_c} = 0$ . The latter relation coupled with formula (13) yields

$$\sigma_c = \frac{2f}{d} + \frac{1}{bS_{sf} \cos \alpha \sin \alpha} \left\{ Db^2 \left[ \frac{d}{2} \ln \frac{|d/2 - p|}{d/2 + \sqrt{p(d-p)}} + \sqrt{p(d-p)} \ln \frac{2p(d-p)}{|d/2 - p|b} \right] + \gamma_{sf} S_{sf} + \beta\gamma S_{step} \right\}. \quad (14)$$

It should be noted that the critical stress  $\sigma_c$  gives only the sufficient condition for dislocation formation at the twin boundary and assumes that the dislocation can overcome the energetic barrier for its nucleation from the nanowire free surface. At the same time, dislocation nucleation requires that the applied load  $\sigma_0$  should be higher than some critical stress  $\sigma'$ . Also, as the applied tensile load  $\sigma_0$  approaches very high values close to the ideal theoretical strength, the stress  $\sigma_c$  becomes higher than the critical stress  $\sigma''$  for the homogeneous generation of a dislocation dipole in the limited space between twin boundaries [3,10]. Thus, formula (14) adequately describes the critical stress for dislocation formation in the interval  $\sigma' < \sigma_0 < \sigma''$ , while at  $\sigma_0 < \sigma'$  or  $\sigma_0 > \sigma''$  the critical stress for dislocation formation in the nanowire should not considerably depend on twin thickness  $h$ .

Using formula (14), we calculate the critical stress  $\sigma_c$  for the case of a gold nanowire characterized by the following parameter values:  $G = 27$  GPa,  $\nu = 0.44$ ,  $\gamma = 1.48$  J/m<sup>2</sup> [38],  $\gamma_{sf} = 0.033$  J/m<sup>2</sup> [42],  $f = 1.4$  J/m<sup>2</sup> [43] and  $\beta = 0.5$ . Recent experiment [10] shows that the critical stress for dislocation formation in a twinned nanowire can be described by a Hall–Petch type relation. Therefore, to make a comparison with this experiment, in Fig. 3a, we plotted the critical stress  $\sigma_c$  vs  $h^{1/2}$ , for various values of the nanowire diameter. Fig. 3a clearly demonstrates that the dependences  $\sigma_c(h^{1/2})$  are very close to linear ones and, thus, can be approximated by Hall–Petch type dependences. Fig. 3 also shows that the theoretical curve  $\sigma_c(h^{1/2})$  that corresponds to the nanowire diameter  $d = 12$  nm perfectly matches experimental points [10] (shown by triangles) in the interval of stresses between 3 and 4 GPa. The upper experimental point that corresponds to the critical stress of 4.2 GPa deviates from the theoretical curve to the region of smaller twin thicknesses because at this stress (close to the ideal theoretical strength of gold) a transition occurs from surface dislocation nucleation to the homogeneous dislocation nucleation inside the nanowire [3,10], and the critical stress for dislocation formation stops to depend on twin thickness. Also, the left experimental point



**Fig. 3.** The dependences of the critical stress  $\sigma_c$  for dislocation formation in a twinned gold nanowire on the parameters (a)  $h^{-1/2}$  and (b)  $d^{-1}$ , where  $h$  and  $d$  are the twin thickness and nanowire diameter, respectively. The dependences are plotted for various values of the nanowire diameter  $d$  (a) and twin thickness  $h$  (b). The triangles represent experimental data from Ref. [10] with the nanowire diameter of 12 nm.

deviates from the corresponding theoretical curve to the region of higher stresses. The possible reason is that the left experimental point corresponds to the case  $\sigma = \sigma'$ , at which the critical stress for dislocation formation stops to depend on twin thickness. At the same time, the discrepancy can also be related to the difference between the model straight dislocation line and its real curved shape, which can result in a slightly higher slope of the calculated  $\sigma_c(h^{-1/2})$  dependence than it should be in reality. In any case, in spite of a slight discrepancy between our model predictions and experimental results [10], Fig. 3a confirms two experimentally revealed trends: (i) the critical stress for dislocation formation in a twinned gold nanowire monotonously increases with decreasing twin thickness, and (ii) in the twin thickness interval between 3 and 8 nm, the dependence of the critical stress for dislocation formation on twin thickness has a Hall–Petch type behavior.

Fig. 3b depicts the dependences of the critical stress  $\sigma_c$  on the inverse of the nanowire diameter,  $d^{-1}$ , for various twin thicknesses. It is seen that  $\sigma_c$  increases with a decrease in the nanowire diameter  $d$  and the dependences  $\sigma_c(d^{-1})$  are close to linear ones, in accord with the results [17] of molecular dynamics simulations. Thus, similar to single crystalline nanowires, twinned nanowires become stronger as their diameter diminishes.

#### 4. SUMMARY

To summarize, by using mechanistic modeling, we have studied the effects of twin thickness and nanowire diameter on the critical stress for dislocation formation in twinned nanowires, which serves

as a lower limit for the nanowire yield strength. Within our model, the twin thickness dependence of the critical stress is associated with the nanowire surface effects, which incorporate dislocation attraction to the nanowire surface, the presence of surface stresses and the formation of surface steps in the course of dislocation nucleation. We have demonstrated that the critical stress for dislocation formation increases with decreasing twin thickness and the dependence of the critical stress on twin thickness has a Hall–Petch type behavior, in agreement with recent experimental observation [10]. This provides the possibilities for the fabrication of superstrong twinned nanowires by reducing their twin thickness.

#### ACKNOWLEDGEMENTS

This work was supported by the Russian Ministry of Education and Science (grant MD-2893.2015.1 and Zadanie № 9.1964.2014/K), St. Petersburg State University (research grant 6.37.671.2013) and the Russian Fund of Basic Research (grant 15-31-20095).

#### REFERENCES

- [1] G. Katopu and O. Yalçın, In: *Nanotechnology and nanomaterials*, ed. by Nicoleta Lupu (InTech, 2010), p. 113.
- [2] R.E. Algra, M.A. Verheijen, M.T. Borgström, L.F. Feiner, G. Immink, W.J.P. van Enckevort, E. Vlieg and E.P.A.M. Bakkers // *Nature* **456** (2008) 369.
- [3] L. Wang, P. Liu, P. Guan, M. Yang, J. Sun, Y. Cheng, A. Hirata, Z. Zhang, E. Ma, M. Chen and X. Han // *Nat. Commun.* **4** (2013) 2413.

- [4] L. Wang, Y. Lu, D. Kong, L. Xiao, X. Sha, J. Sun, Z. Zhang and X. Han // *Acta Mater.* **90** (2015) 194.
- [5] T.C. Chen, Y.M. Lin, H.W. Tsai, Z.M. Wang, C.N. Liao and Y.L. Chueh // *Nanoscale* **6** (2014) 7332.
- [6] L. Lu, Y.F. Shen, X.H. Chen, L.H. Qian and K. Lu // *Science* **304** (2004) 422.
- [7] K. Lu, L. Lu and S. Suresh // *Science* **324** (2009) 349.
- [8] L. Lu, X. Chen, X. Huang and K. Lu // *Science* **323** (2009) 607.
- [9] J. Wang, F. Sansoz, J. Huang, Y. Liu, S. Sun, Z. Zhang and S.X. Mao // *Nat. Com.* **4** (2013) 1742.
- [10] J. Wang, F. Sansoz, C. Deng, G. Xu, G. Han and S.X. Mao // *Nano Lett.* **15** (2015) 3865.
- [11] K.A. Afanasyev and F. Sansoz // *Nano Lett.* **7** (2007) 2056.
- [12] A.J. Cao, Y.G. Wei and S.X. Mao // *Appl. Phys. Lett.* **90** (2007) 151909.
- [13] M.T. McDowell, A.M. Leach, K. Gaill // *Nano Lett.* **8** (2008) 3613.
- [14] Y.F. Zhang, H.C. Huang and S.N. Atluri // *Comp. Model. Eng. Sci.* **35** (2008) 215.
- [15] Y. Kulkarni and R.J. Asaro // *Acta Mater.* **57** (2009) 4835.
- [16] C. Deng and F. Sansoz // *Nano Lett.* **9** (2009) 1517.
- [17] C. Deng and F. Sansoz // *Appl. Phys. Lett.* **95** (2009) 091914.
- [18] C. Deng and F. Sansoz // *ACS Nano* **3** (2009) 3001.
- [19] C. Deng and F. Sansoz // *Acta Mater.* **57** (2009) 6090.
- [20] X. Guo and Y.Z. Xia // *Acta Mater.* **59** (2011) 2350.
- [21] D. Jang, X. Li, H. Gao and J.R. Greer // *Nat. Nanotechnol.* **7** (2012) 594.
- [22] Y.H. Wen, R. Huang, Z.Z. Zhu and Q. Wang // *Comput. Mater. Sci.* **55** (2012) 205.
- [23] Z.X. Wu, Y.W. Zhang, M.H. Jhon, J.R. Greer and D.J. Srolovitz // *Acta Mater.* **61** (2013) 1831.
- [24] F. Hammami and Y. Kulkarni // *J. Appl. Phys.* **116** (2014) 033512.
- [25] Y. Gao, Y. Sun, Y. Yang, Q. Sun and J. Zhao // *Molecular Simulations* (2015), doi: 10.1080/08927022.2014.999238
- [26] T. Zhu, J. Li, A. Samanta, A. Leach and K. Gall // *Phys. Rev. Lett.* **100** (2008) 025502.
- [27] C. Peng, Y. Zhong, Y. Lu, S. Narayanan, T. Zhu and J. Lou // *Appl. Phys. Lett.* **102** (2013) 083102.
- [28] L.B. Freund, S. Suresh, *Thin Film Materials: Stress, Defect Formation, and Surface Evolution* (Cambridge University Press, Cambridge, 2004).
- [29] M.Yu. Gutkin, I.A. Ovid'ko and A.G. Sheinerman // *J. Phys.: Condens. Matter* **12** (2000) 5391.
- [30] A.G. Sheinerman and M.Yu. Gutkin // *Phys. Stat. Solidi A* **184** (2001) 485.
- [31] I.A. Ovid'ko and A.G. Sheinerman // *Phil. Mag.* **84** (2004) 2103.
- [32] F. Glas // *Phys. Rev. B* **74** (2006) 121302(R).
- [33] K.E. Aifantis, A.L. Kolesnikova and A.E. Romanov // *Phil. Mag.* **87** (2007) 4731.
- [34] M. Yu. Gutkin and A.M. Smirnov // *Acta Mater.* **88** (2015) 91.
- [35] S.V. Bobylev and I.A. Ovid'ko // *Phys. Rev. B* **83** (2011) 054111.
- [36] S.V. Bobylev and I.A. Ovid'ko // *Phys. Rev. Lett.* **103** (2009) 135501.
- [37] I.A. Ovid'ko // *Phys. Rev. Lett.* **88** (2002) 046103.
- [38] J.P. Hirth and J. Lothe, *Theory of Dislocations* (Wiley, New York, 1982).
- [39] I.N. Bronshtein and K.A. Semendyaev, *Reference book on Mathematics* (Moscow, 1954), In Russian.
- [40] R.C. Cammarata // *Prog. Surf. Sci.* **46** (1994) 1.
- [41] W. Zhang, T. Wang and X. Chen // *J. Appl. Phys.* **103** (2008) 123527.
- [42] S. Kibey, J. B. Liu, D. D. Johnson and H. Sehitoglu // *Acta Mater.* **55** (2007) 6843.
- [43] V.B. Shenoy // *Phys. Rev. B* **71** (2005) 094104.