University of Groningen

Strain rate effects on the plastic flow in submicron copper pillars

Hu, Jianqiao; Liu, Zhanli; Van der Giessen, Erik; Zhuang, Zhuo

Published in:
Extreme Mechanics Letters

DOI:
[10.1016/j.eml.2017.09.011](https://doi.org/10.1016/j.eml.2017.09.011)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2017

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Hu, J., Liu, Z., Van der Giessen, E., & Zhuang, Z. (2017). Strain rate effects on the plastic flow in submicron copper pillars: Considering the influence of sample size and dislocation nucleation. *Extreme Mechanics Letters*, 17, 33-37. <https://doi.org/10.1016/j.eml.2017.09.011>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Strain rate effects on the plastic flow in submicron copper pillars: Considering the influence of sample size and dislocation nucleation

Jianqiao Hu^a, Zhanli Liu^a, Erik Van der Giessen^{b,*}, Zhuo Zhuang^{a,*}

^a Applied Mechanics Lab., School of Aerospace Engineering, Tsinghua University, Beijing 100084, China

^b Zernike Institute for Advanced Materials, Department of Applied Physics, University of Groningen, Nyenborgh 4, 9747 AG Groningen, The Netherlands

GRAPHICAL ABSTRACT

ARTICLE INFO

Article history:

Received 14 July 2017

Accepted 26 September 2017

Available online 9 October 2017

Keywords:

Dislocation mechanisms

Stable flow stress

Surface nucleation

Strain rate effect

ABSTRACT

Three-dimensional discrete dislocation dynamics (DDD) simulations are performed to investigate the plastic flow behaviors of submicron copper pillars under different loading rates, in which both inertial effect of dislocation motion and surface nucleation are taken into account. It is found that: (1) for pillars with a diameter below ~ 400 nm, there is a transition from internal dislocation multiplication to surface dislocation nucleation as the strain rate increases ($\geq 10^4$ s⁻¹); (2) for ~ 1 μm diameter pillars, stable internal dislocation sources dominate for both low and high strain rates; (3) in general, a larger strain rate, smaller sample size and less internal dislocation sources make it more probable for a surface nucleation process to take the place of dislocation multiplication. Furthermore, a theoretical model is proposed to predict the submicron plastic behavior at different strain rates when internal dislocation sources prevail.

© 2017 Elsevier Ltd. All rights reserved.

1. Introduction

It is well known that various aspects of mechanical behavior at submicron scales are quite different from those at the bulk scale. In addition to the widely known plasticity size effect [1–3], strain rate sensitivity at submicron scale has attracted much attention [4–6].

Recently, Jennings et al. [7] demonstrated strain rate effect emerging in the single crystalline copper pillars at submicron scales by experiments. By computing the activation volumes, as a function of pillar diameter at each strain rate, they postulated a plasticity mechanism transition from dislocation multiplication via the operation of single-arm sources to surface dislocation nucleation when the pillar size became smaller. The effects of both strain rate and sample size on the compressive strength of single crystalline copper were reported in their work while the quantitative investigations of dislocation sources and structures were quite

* Corresponding authors.

E-mail addresses: e.van.der.giessen@rug.nl (E. Van der Giessen), zhuangz@tsinghua.edu.cn (Z. Zhuang).

limited. Lately, Gurrutxaga-Lerma et al. [8] investigated the dominant dislocation mechanism at different strain rates ranging from 10^1 s^{-1} to 10^{10} s^{-1} and illustrated the strain rate effect on both the activation time and the source strength of Frank–Read sources. They discussed Frank–Read sources and homogeneous nucleation processes which are essential in bulk deformation. However, in submicron and nano-sized samples, dislocation nucleation from the free surface has been observed to be a potent mechanism, e.g. [7,9].

Discrete dislocation dynamics (DDD) simulations have been reported in the literature that provide important insights into the mechanical behavior under different strain rates. They served as an effective method to study the dislocation based plasticity under low strain rates [10], high strain rates [11–14] and extremely high strain rates as shock compression [15–17]. The calculation procedure always follows the same general form. The forces acting on all the dislocation segments are evaluated at each time step, dislocation velocities are calculated by solving the equations of motion, and dislocation positions are updated for the next time step. In most applications of the DDD simulations, the equation of dislocation motion involves a linear force–velocity law, instead of the full dynamical formula which includes inertia. This assumption seems sufficient to describe dislocation motion at low deformation rates, but may be not appropriate in high strain rate deformation. Wang et al. [18] employed a full dynamical equation of dislocation motion to compare with the commonly assumed linear force–velocity dynamics. Through comparison and analysis, they indicated the inertial effect could not be ignored when the strain rate was 10^4 s^{-1} and larger.

In this paper, the plastic flow behavior of single crystalline copper pillars is investigated by 3D DDD simulations. We concentrate on the combined effect of sample size, strain rate and surface versus internal sources of dislocations on the mechanical behavior at submicron scales.

2. Methodology

The 3D DDD method used here has been described in detail in our previous paper [19]. Compared to the conventional DDD model, two new features are introduced. A full dynamical equation of dislocation motion including inertial effect is adopted and surface nucleation process is introduced.

The full dynamical equation of dislocation motion is

$$m_e \ddot{v} + Bv = f, \quad (1)$$

where m_e is the effective mass of dislocation per unit length, $m_e = \rho_c b^2$, ρ_c is the material density and b is the magnitude of the Burgers vector. B is the viscous drag coefficient, f is the total Peach–Koehler force of the applied stress and interaction with other defects, line tension, as well as the image force by the free surface.

The introduction of dislocation sources associated with surface nucleation in the DDD computations is motivated by the atomistic model of Zhu et al. [20]. Their results suggest the free surface acts as an effective source of dislocations and the nucleation stress provides an upper bound to the strength of compressive nanopillars. Their probabilistic investigations revealed that the probability of dislocation nucleation from the free surface within a time span dt is given by

$$P = v_0 \exp \left[-\frac{Q(\sigma, T)}{k_B T} \right] \times \left(\frac{S}{b^2} \right) \times dt. \quad (2)$$

Here, v_0 is the attempt frequency, $Q(\sigma, T)$ is the activation free energy of dislocation nucleation from the free surface and $k_B T$ is the thermal energy, $\frac{S}{b^2}$ is the number of nucleation sites at the surface. In the DDD simulations, we expand the possible nucleation sites from sample corner to the whole surface, dislocation can

nucleate at any point on the surface of the pillar and the stress $\sigma = |\sigma_{33}|$ is used in the simulations of compression test. A first approximation of the temperature effect on the activation free energy is introduced as

$$Q(\sigma, T) = \left(1 - \frac{T}{T_m} \right) \cdot Q_0(\sigma), \quad (3)$$

where T_m is the surface disordering temperature and is chosen to be 700 K. By taking the function form $Q_0(\sigma) = A(1 - \sigma/\sigma_{ath})^\alpha$ to fit the calculated activation energies at different stresses, $A = 4.8 \text{ eV}$, $\sigma_{ath} = 5.2 \text{ GPa}$, and $\alpha = 4.1$ are obtained [20]. The probability of surface nucleation is calculated at each time span. The number of nucleated dislocations N is as follows

$$N = \begin{cases} \text{Integer}[P], & \text{if } \int_{t_m}^{t_n} P \geq 1 \\ 0, & \text{if } \int_{t_m}^{t_n} P < 1. \end{cases} \quad (4)$$

Here, the probability of dislocation nucleation is accumulated from t_m to t_n because that once a dislocation nucleation process occurs, the probability starts from zero again, and an arc-shaped dislocation loop on a random slip system of all the twelve typical FCC is introduced at a stochastic site on the surface.

In the simulations, the cross sections of single crystalline copper pillars are set to be square. Side lengths are varied from 200 to 800 nm while the ratio of pillar height H to side length D is fixed to 2. These cuboid cells are used to mimic the cylindrical specimens used in the experiment [21], because it is easier to deal with the image force and it is known that the cross-section shape has only a weak effect [22]. All the pillars are loaded along (001) direction in a displacement-controlled manner and the lateral surfaces are traction free. A wide range of strain rates are performed in DDD simulation, ranging from 10^4 s^{-1} to 10^6 s^{-1} . The initial dislocation densities are around $4 \times 10^{13} \text{ m}^{-2}$. The simulation for each pillar size is carried out for five different initial dislocation distributions to illustrate the stochastic scatter. The material properties of copper are as follows: shear modulus μ is 48 GPa, Poisson's ratio ν is 0.34, the density of Cu $\rho_c = 8.96 \times 10^3 \text{ kg/m}^3$, and the viscous drag coefficient $B = 2 \times 10^{-5} \text{ Pa s}$. The attempt frequency v_0 in Eq. (2) is set at 10^{13} s^{-1} [23] and the temperature $T = 300 \text{ K}$. The time step used in the simulations is $\Delta t = 10^{-12} \text{ s}$ which ensures that the numerical results are converged.

3. Results and discussions

The simulation results of pillars with different side lengths are shown in Fig. 1(a). The stress–strain curves exhibit three typical characteristics. For type I which is generally observed in small pillars ($D < 400 \text{ nm}$), as marked in Fig. 1(a), the stress increases in an elastic way at the initial stage, then early yield events that are of short duration occur at various stress levels (varying between ~ 500 and $\sim 1200 \text{ MPa}$), followed by an extensive elastic period, after which massive yield takes place at a stress level of around 1600 MPa. Despite the small oscillation, the flow stress is approximately stable in the end. Distinct from this, in type III plasticity, yield is massive right away and the stress remains roughly stable without obvious strain hardening. As a result, the flow stress is relatively low comparing with that in type I. Type II falls in between type I and III, it seems the stress remains stable after the initial yielding, but strain hardening can start at an unexpected time.

The evolution of representative dislocation structures corresponding to type I and III is shown in Fig. 1(b). For pillars as small as 200 nm, it is difficult for dislocations to form stable pinning points, and the initial dislocations will be driven out quickly by the subsequent external loading. After that, new dislocations emerge

Fig. 1. (a) Stress–strain curves for pillars with different size at an applied strain rate of 10^6 s^{-1} , (b) typical dislocation structures for type I and III.

Fig. 2. Stress–strain curves for pillars with different size at strain rates from 10^4 s^{-1} to 10^6 s^{-1} , (a) $D = 200 \text{ nm}$; (b) $D = 800 \text{ nm}$.

from the free surface and escape immediately out of the pillar. The small oscillation of flow stress is attributed to the repeated nucleation and escape of surface dislocations. It is therefore a surface nucleation dominant mechanism in small pillars, characterized by very high flow stress. In large pillars ($D = 800 \text{ nm}$) as type III, by contrast, the internal dislocations can self-organize to form jammed configuration initially. With the increase of external loading, the jammed network will continuously evolve until internal dislocation sources with stable pinning points are formed. Both single-arm sources and Frank–Read sources exist inside large pillars at the moment. The operation of these internal sources can generate enough plasticity and keep the flow stress stable. In this case, the dislocation multiplication mechanism plays a leading role, featuring relative low stress levels. The mechanical behavior of medium-sized pillars ($D = 400\text{--}600 \text{ nm}$) is quite sensitive to the initial dislocation configuration. For those samples without enough dislocation junctions and tangles, after the break of weak links between dislocations, only a few single-arm sources are formed inside the pillars and their operation leads to a provisional yielding stage. However, the dislocation sources can become progressively exhausted, causing dislocation starvation hardening as type II in Fig. 1(a).

In addition to the sample size, the strain rate also has a significant effect on the plastic behavior. To investigate the effects of strain rate, imposed by different displacement rates at the pillar ends, stress–strain curves for pillars with side lengths 200 and 800 nm are shown in Fig. 2, respectively. Two distinct types of plastic

behavior are observed, distinguished by different stress levels. For small pillars ($D = 200 \text{ nm}$), the flow stresses are generally high within the investigated range of strain rates ($\geq 10^4 \text{ s}^{-1}$). Just as type I as shown in Fig. 1(b), all initial dislocations tend to escape out due to external loading. Then the surface nucleation takes over as the dominant dislocation mechanism since there are no pre-existing dislocations left. Moreover, dislocation starvation and surface nucleation are more likely to happen with the increase of strain rate. Nevertheless, in a small number of pillars with side length 200 nm, one or a few stable single-arm sources may persist at relative low strain rates. The operation of these sources can also result in a relatively low flow stress like in large pillars. In contrast, as shown in Fig. 2(b), the flow stress in large pillars ($D = 800 \text{ nm}$) is generally not high enough for dislocation nucleation from the surface to be activated.

The exhaustion of internal sources leads to an elastic stress increase and results in the surface nucleation process eventually. The stable flow stresses which involve in nucleation process, characterized by the absence of a hardening process, can be predicted by the surface nucleation formula. In case of the dislocation multiplication dominated process, the stable flow stresses vary greatly even in the case of same strain rate and sample size, as shown in Fig. 2(b). We systematically investigated the evolution of internal dislocation structures and found that internal source-controlled yield is controlled just by the number of internal dislocation sources. Consequently, the stable flow stress also depends on the number of dislocation sources besides sample size and strain

Fig. 3. (a) Stress–strain curves for pillars with same size ($D = 800$ nm) and strain rate ($\dot{\epsilon} = 1 \times 10^6 \text{ s}^{-1}$), (b) Dislocation structures corresponding to each marked points in (a).

Table 1
Comparison of simulation and analytical solution between two pillars.

	Number of single-arm sources n at			Simulated flow stress (MPa)	Analytical prediction (value of n)
	A_1 or B_1	A_2 or B_2	A_3 or B_3		
Pillar 1	8	7	9	509	534 MPa (8)
Pillar 2	13	9	12	444	451 MPa (11)

rates. Following [3,19,24], we here propose the following formula for the stable shear flow strength associated with the three factors:

$$\tau = \underbrace{\tau_0 + \alpha \mu b \sqrt{\rho}}_{\tau_{\text{static}}} + \frac{k \mu b}{\lambda} + \frac{B \dot{\epsilon} V}{M b^2 \lambda \cdot n}. \quad (5)$$

Here, the first three items on the right-hand side are the internal source-controlled critical resolved shear stress under quasi-static loading, as systematically studied by Cui et al. [19], τ_0 is the lattice friction stress, α and k are dimensionless constants, usually α is set at 0.5 and k is taken as 1.0 in previous literatures [3,24], ρ is the dislocation density and λ is the average effective source length. The last term is an additional part due to the strain rate effect, in which, $\dot{\epsilon}$ is the strain rate, V is sample volume, n is the number of stable single-arm sources, M is Schmid factor. Obviously, the contribution of the last term increases when the strain rate becomes higher. In particular, for pillars with adequate internal dislocation sources, the last item in Eq. (5) can be neglected as $n \rightarrow \infty$ (except when strain rate $\dot{\epsilon} \rightarrow \infty$) and the stable flow strength reduces to the quasi-static one. It possesses a physical foundation in Orowan's law. Furthermore, for a certain strain rate loading, the stress obtained in Eq. (5) could become high enough to trigger the surface nucleation if the source number n is quite limited. Once the shear flow strength is obtained by Eq. (5), the flow stress can be calculated by $\sigma = \tau / M$, where M is the Schmid factor.

In order to test the above proposition, especially the effect of the number of dislocation sources, the results for two pillars with side length 800 nm are investigated in detail. For each case, the dislocation configuration at three strain levels well into the plastic regime are considered, see Fig. 3. During the analysis, the stable flow stress is calculated by averaging all the stress values within the strains ranging from 1.2% to 1.6% in the simulation to eliminate the influence of stress oscillation. It can be seen clearly that more dislocation sources in Pillar 2 result in a relatively low flow stress. The stable flow stresses are given in Table 1 for two pillars by numerical simulation and analytical solution. The analytical solutions are consistent with the simulation results.

Fig. 4. Dislocation mechanism map for plastic flow at submicron scales: nucleation of surface dislocations (Type I), cooperation of dislocation multiplication and surface nucleation (Type II) and stable internal single-arm dislocation multiplication (Type III).

In addition, it is worth pointing out that the analytical solution we achieved is based on the single-arm source dominant mechanism, which is suitable at submicron scales but not for very small or very large sample size. TEM experiments [25] have revealed that the pillars with diameter smaller than 160 nm can achieve dislocation starvation by mechanical annihilation. Through the above analysis, a schematic diagram of the governing dislocation mechanisms in plastic deformation at submicron scales which unifies the three combined effects can be presented in Fig. 4, in which the mechanisms are divided into three zones that depend on the sample size D , strain rate $\dot{\epsilon}$ and stable dislocation density ρ_s or source number n . The three zones are corresponding to the three types in Fig. 1. Several characteristic values for the transitions extracted from the computations in this work are also marked in Fig. 4.

4. Conclusions

To summarize, the effects of sample size, strain rate and dislocation sources on the plastic behavior of pillars with a diameter roughly between 100 nm and 1 μm are investigated by DDD simulations. In small pillars (~ 200 nm), dislocation pinning points are not formed and the initial dislocations run across the sample and escape out easily. Dislocation starvation triggers nucleation of dislocations from the surface, which gives rise to a very high stable flow stress. In contrast, at the same initial dislocation density, dislocations in large pillars have a smaller tendency to escape from the free surface and more probability to develop stable pinning points. As a result, the plastic behavior of large pillars is always dominated by dislocation multiplication, featuring relatively low stress levels. At higher strain loading rates, the flow stress tends to increase because the limited number of internal sources cannot generate enough plasticity to resist the increment of external loading, that is $\dot{\epsilon}^p < \dot{\epsilon}$. In turn, these internal dislocation sources may be broken due to the increasing stress. Finally, to illustrate the central role of stable dislocation sources, an analytical expression is proposed to compare with the simulation results and further explains why the stable flow stress varies even in pillars with same size and strain rate. We emphasize the role of stable dislocation sources but not the initial dislocation density since it directly translates into the probability to achieve stable internal dislocation sources.

Acknowledgments

This work is supported by the Key Program of National Natural Science Foundation of China (NSFC) through Grant No. 11132006 and 11302115. The support from the Sino-Dutch Scholarship Programme is gratefully acknowledged.

References

- [1] J.R. Greer, W.C. Oliver, W.D. Nix, *Acta Mater.* 53 (2005) 1821–1830.
- [2] J.R. Greer, W.D. Nix, *Phys. Rev. B* 73 (2006) 245410.
- [3] T.A. Parthasarathy, S.I. Rao, D.M. Dimiduk, M.D. Uchic, D.R. Trinkle, *Scr. Mater.* 56 (2007) 313–316.
- [4] H. Zhang, X. Dong, D. Du, Q. Wang, *Mater. Sci. Eng. A* 564 (2013) 431–441.
- [5] Z.L. Liu, X.C. You, Z. Zhuang, *Int. J. Solids Struct.* 45 (2008) 3674–3687.
- [6] A.S. Khan, J. Liu, J.W. Yoon, R. Nambori, *Int. J. Plast.* 67 (2015) 39–52.
- [7] A.T. Jennings, J. Li, J.R. Greer, *Acta Mater.* 59 (2011) 5627–5637.
- [8] B. Gurrutxaga-Lerma, D.S. Balint, D. Dini, A.P. Sutton, *J. Mech. Phys. Solids* 84 (2015) 273–292.
- [9] I. Ryu, W. Cai, W.D. Nix, H. Gao, *Acta Mater.* 95 (2015) 176–183.
- [10] H.M. Zbib, T. Diaz de la Rubia, *Int. J. Plast.* 18 (2002) 1133–1163.
- [11] A. Roos, J.T.M. De Hosson, E. Van der Giessen, *Comput. Mater. Sci.* 20 (2001) 19–27.
- [12] A. Roos, J.T.M. De Hosson, E. Van der Giessen, *Comput. Mater. Sci.* 20 (2001) 1–18.
- [13] Z.Q. Wang, I.J. Beyerlein, R. Lesar, *Phil. Mag.* 88 (2008) 1321–1343.
- [14] P.K. Agnihotri, E. Van der Giessen, *Mech. Mater.* 90 (2015) 37–46.
- [15] M.A. Shehadeh, H.M. Zbib, T. Diaz de la Rubia, *Int. J. Plast.* 21 (2005) 2369–2390.
- [16] M. Kattoura, M.A. Shehadeh, *Phil. Mag. Lett.* 94 (2014) 415–423.
- [17] M.A. Shehadeh, *Phil. Mag.* 92 (2012) 1173–1197.
- [18] Z.Q. Wang, I.J. Beyerlein, R. Lesar, *Phil. Mag.* 87 (2007) 2263–2279.
- [19] Y. Cui, P. Lin, Z. Liu, Z. Zhuang, *Int. J. Plast.* 55 (2014) 279–292.
- [20] T. Zhu, J. Li, A. Samanta, A. Leach, K. Gall, *Phys. Rev. Lett.* 100 (2008) 025502.
- [21] S.I. Rao, D.M. Dimiduk, T.A. Parthasarathy, M.D. Uchic, M. Tang, C. Woodward, *Acta Mater.* 56 (2008) 3245–3259.
- [22] D. Kiener, P.J. Guruprasad, S.M. Keralavarma, G. Dehm, A.A. Benzerga, *Acta Mater.* 59 (2011) 3825–3840.
- [23] S. Ryu, K. Kang, W. Cai, *J. Mater. Res.* 26 (2011) 2335–2354.
- [24] S.-W. Lee, W.D. Nix, *Phil. Mag.* 92 (2012) 1238–1260.
- [25] Z.W. Shan, R.K. Mishra, S.A. Syed Asif, O.L. Warren, A.M. Minor, *Nat. Mater.* 7 (2008) 115–119.