Metallophysics and Advanced Technologies
Металофіз. новітні технол.
Metallofiz. Noveishie Tekhnol.
2026, vol. 48, No. 9, pp. 931–947
https://doi.org/10.15407/mfint.48.09.0931
Reprints available directly from the publisher

© 2026 G. V. Kurdyumov Institute for Metal Physics,
National Academy of Sciences of Ukraine
Published by license under
the G. V. Kurdyumov Institute for Metal Physics–
N.A.S. of Ukraine Publishers imprint.
Printed in Ukraine.

PACS numbers: 05.40.-a, 61.72.Bb, 61.72.Lk, 62.20.F-, 62.25.Fg, 83.50.-v, 83.60.-a

Length of a Critical Dislocation Segment under the Influence of Thermal Fluctuations

M. I. Lugovy, D. G. Verbylo, M. P. Brodnikovskyy, T. I. Verbytska*, D. S. Leonov**, and M. Yu. Barabash*,**,***,****

I. M. Frantsevich Institute for Problems in Materials Science, N.A.S. of Ukraine,
3 Omeljan Pritsak Str.,
UA-03142 Kyiv, Ukraine
**National Technical University of Ukraine*
'Igor Sikorsky Kyiv Polytechnic Institute',
37 Beresteiskyi Ave.,
UA-03056 Kyiv, Ukraine
***Technical Centre, N.A.S. of Ukraine,*
13 Pokrovs'ka Str.,
UA-04070 Kyiv, Ukraine
****Institute for Applied Control Systems, N.A.S. of Ukraine,*
42 Academician Hlushkov Ave.,
UA-03187 Kyiv, Ukraine
*****Gas Institute, N.A.S. of Ukraine,*
39 Dehtyarivs'ka Str.,
UA-03113 Kyiv, Ukraine

The thermal motion of atoms and, in other words, thermal fluctuations or distortions of crystal lattice caused by this motion lead to a wavy shape of the dislocation line both in alloys, where there are dissolved atoms, and in pure metals, where there are no such atoms. The wavy shape of the dislocation line, in turn, indicates that there are obstacles to the movement of the dislocation in the material. This means the threshold stress to initiate the disloca-

Corresponding author: Tetyana Ivanivna Verbytska
E-mail: verbutska@gmail.com

Citation: M. I. Lugovy, D. G. Verbylo, M. P. Brodnikovskyy, T. I. Verbytska, D. S. Leonov, and M. Yu. Barabash, Length of a Critical Dislocation Segment under the Influence of Thermal Fluctuations, *Metallofiz. Noveishie Tekhnol.*, **48**, No. 9: 931–947 (2026). DOI: 10.15407/mfint.48.09.0931

© Publisher PH 'Akademperiodyka' of the NAS of Ukraine, 2026. This is an open access article under the CC BY-ND license (https://creativecommons.org/licenses/by-nd/4.0)

tion movement could be very probable. In such a way, the dislocation line shape can affect the yield strength of the metal or alloy. The interaction of thermal fluctuation with a dislocation is considered as kind of 'push' into the dislocation of an atom in thermal motion. The dislocation-line shape under thermal-fluctuations' action is determined by the discrete dislocation dynamics method and in the form of an analytical solution of the differential equation for an elastic string with fixed ends. The standard deviation of dislocation-line points from the straight line and the averaged bulge length under thermal fluctuations action, determined by discrete dislocation dynamics and the analytical method, correlate well with each other, confirming the reliability of the modelling results. The standard deviation increases in proportion to the square root of the dislocation-line length at constant temperature and is also proportional to the square root of the temperature at constant dislocation-line length. The averaged bulge length, which determines the critical dislocation-segment length, is directly proportional to the dislocation-line length at constant temperature and does not depend on temperature at constant dislocation-line length.

Key words: dislocation, shear stress, standard deviation, length of the critical dislocation segment, thermal fluctuations.

Розглянуто вплив термічних флюктуацій на форму лінії дислокації. Взаємодія термічної флюктуації з дислокацією розглядається як своєрідний «поштовх» у неї атому, який перебуває в тепловому русі. Форму лінії дислокації під дією термічних флюктуацій визначено, з одного боку, за допомогою дискретної дислокаційної динаміки та, з іншого боку, у вигляді аналітичного рішення загального диференційного рівняння для пружньої струни з закріпленими кінцями. Запропоновано спосіб розрахунку характеристик «хвилястости» лінії дислокації, яку викликано термічними флюктуаціями. Цей спосіб уможливлює розраховувати стандартний відхил точок лінії дислокації від прямої та довжину усередненої випуклости на ній. Довжина усередненої випуклости визначає довжину критичного сеґмента дислокації. Показано, що характеристики, розраховані аналітичною методою та за допомогою комп'ютерного моделювання методою дискретної дислокаційної динаміки, добре корелюють між собою. Визначено також температурні залежності цих характеристик. Стандартний відхил пропорційний кореню квадратному з температури, а довжина критичного сеґмента від температури не залежить.

Ключові слова: дислокація, зсувне напруження, стандартний відхил, довжина критичного сеґмента, термічні флюктуації.

(Received 12 August, 2026; in final version, 17 August, 2026)

1. INTRODUCTION

Thermal fluctuations, thermal motions of atoms are present in all materials. They affect the shape of the dislocation line. This line cannot maintain a straight shape under such conditions and becomes wavy [1].

The shape of the dislocation line, in turn, can affect the formation of the yield point of a metal or alloy. The yield point is an important mechanical characteristic of metal alloys from the point of view of their engineering applications. Among various alloys, multicomponent alloys can be distinguished as particularly promising [2, 3]. The study of solid solution strengthening—the basic mechanism for increasing the yield point of such alloys—has been the subject of many works in the past [4–12]. In addition, attention has been paid to the temperature dependence of the yield point of alloys both theoretically [13–23] and experimentally [24–26]. Various aspects of the thermal activation motion of dislocations and the temperature dependence of the yield point were also studied in [27–30]. The calculation of solid solution strengthening of multicomponent heat-resistant alloys [31, 32] and the determination of crystal lattice distortion [33] are also important. Modelling the shear stress field in the glide plane in a substitutional solid solution and the movement of dislocations in this field provides new opportunities in such studies [34–37]. The temperature dependence of the yield point in an alloy can also be determined in terms of two components of the shear stress field in the glide plane [38]. Important issues in this regard remain the method of determining the parameters of the shear stress field and the correct description of the dependence of lattice distortion on temperature in a multicomponent alloy [39, 40].

The shape of an elastic line, which is fixed at both ends, under the action of thermal fluctuations at thermal equilibrium was modelled by the method of discrete dislocation dynamics in [1]. In order to investigate the dynamics of the shape change, an initially straight elastic line was considered, which then moved under the action of random thermal forces in the overdamped regime. The coefficient of resistance to the movement of the dislocation was considered directly proportional to the temperature, and the time step was equal to 50 fs. The shapes of the dislocation line were modelled for temperatures of 300, 600, 900 and 1200 K. After a sufficient modelling time, the system reached thermal equilibrium and the average kinetic energy per each degree of freedom became equal to the standard thermodynamic quantity for a given temperature, and the velocities of the discrete elements of the dislocation line had a Maxwell distribution.

In Ref. [1], the transient dynamics of the dislocation line shape before reaching thermal equilibrium was also studied. The initial shape was a straight line, which gradually transformed under the action of thermal fluctuations into a self-similar ‘wavy’ shape. This process was characterized by a structure factor, which was defined as the average absolute value of the difference in coordinates in the direction perpendicular to the initial line of two discrete dislocation elements located at a given distance from each other along this initial line. It is obvious

that, for the initial line, this parameter is zero for all distances between discrete elements along this line. Further, as thermal equilibrium approaches, the dependence of this factor on the distance along the initial line has two characteristic regions. For small distances, this dependence is approximately a straight line on a double logarithmic graph, which corresponds to a self-similar shape. For large distances, this parameter reaches a certain value that does not depend on the distance and essentially determines the width of the 'wavy' line in the direction perpendicular to the initial line. This width gradually increases with time in the transition period until complete thermal equilibrium is achieved. The distance along the initial line along which the transition between the two characteristic regions occurs also increases under these conditions. However, the characteristics of the 'wavy' dislocation line under the action of thermal fluctuations in the state of thermal equilibrium, when these characteristics become independent of time, were not considered in Ref. [1].

The movement of a dislocation occurs by gradually moving its individual critical segments due to the formation and transformation of bulges on them [38]. Therefore, the average length and height of the bulge on the dislocation as parameters of the critical segment are very important for describing the dislocation motion and, mostly, the yield strength of the alloy. In an alloy, in a solid solution, these parameters determine the effective dimensions of the obstacle created by dissolved atoms for such motion [38]. Thermal fluctuations and the distortions associated with them also lead to the 'waviness' of the dislocation line even in the absence of dissolved atoms. Bulges on the dislocation line, which are formed due to the thermal motion of atoms, in contrast to bulges formed under the action of dissolved atoms, are dynamic, not stationary and change with time, but their average length will also determine the length of certain critical segments. It is important that this length be determined in a state of thermal equilibrium, when these characteristics become independent of time.

The goal of this work is to calculate, by analytical method and using computer modelling by the method of discrete dislocation dynamics, the standard deviation of the points of the dislocation line from the straight line and the length of the averaged bulge on it, *i.e.*, the length of the critical dislocation segment, in the case of thermal fluctuations, and to determine the temperature dependences of these characteristics.

2. CALCULATION ALGORITHMS

Consider a dislocation with length l, which is fixed at the ends. We will assume that in the glide plane a coordinate system is given, where the axis x is directed in the direction of dislocation movement, perpendicu-

lar to the dislocation line, and the axis z is in the direction of the dislocation line, *i.e.*, parallel to it. We can discretize the dislocation line, *i.e.*, represent it as a chain of separate segments with the length of each Δz ($\Delta z << 1$), which are parallel to the axis z. We will also assume that each segment interacts with neighbouring segments due to the linear tension force. The equation of motion of such a separate dislocation segment along the axis x under the action of thermal fluctuations can be proposed in a certain approximation in a form similar to the works [1, 34, 37]:

$$m_0 \frac{\partial^2 u_i}{\partial t^2} + B \frac{\partial u_i}{\partial t} - \Gamma \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta z^2} = f_T(z_i, t), \quad (1)$$

where $u_i = u_i(z_i, t)$ is the displacement from the zero position along the coordinate x of the dislocation segment, which has the coordinate of its centre $z_i = \Delta z i$ at the time instant t ($u_i(z_i, t)$ essentially determines the shape of the dislocation line at the time instant t, $i = 1, 2, \ldots, l/\Delta z$), x is the coordinate in the direction of dislocation movement, z is the coordinate in the direction of the dislocation line, xOz is the dislocation glide plane, m_0 is the effective mass of the dislocation per unit length ($m_0 \approx \rho b^2/2$) [1], $m_0 \Delta z$ is the mass of the dislocation segment, ρ is the density of the material, b is the length of the Burgers vector, B is the coefficient of resistance to movement (it can be assumed that this coefficient is directly proportional to the temperature T [1], *i.e.*, $B = qT$, where q is the proportionality coefficient, such an assumption simplifies further consideration and gives a good approximation for temperatures that are not too close to zero), Γ is the linear tension of the dislocation line ($\Gamma = \alpha G b^2$, where α is the coefficient ($0 < \alpha \le 0.5$), G is the shear modulus), $f_T(z_i, t)$ is the force per unit length acting on the dislocation segment from the side of atoms that are in thermal motion, in the direction of the axis x. This force for each segment at each time step Δt in numerical simulation can be given as [1]:

$$f_T(z_i, t) = s_T Z_i, \quad (2)$$

where $s_T = \sqrt{2Bk_BT/(\Delta z \Delta t)}$ is the standard deviation of the force that ensures the existence of thermal equilibrium in the system, when the energy transferred from the atoms to the dislocation segment is returned back to the atoms due to the viscous resistance of the dislocation motion, Z_i is a random variable with a normal probability distribution and a mean value equal to 0 and a variance equal to 1 (a standard normal random variable for each i), k_B is the Boltzmann constant. It should be noted that $(u_{i-1} - 2u_i + u_{i+1})/\Delta z^2$ is the numerical representation of the second partial derivative $\partial^2 u(z, t)/\partial z^2$, which determines the curvature of the dislocation line, the shape of which at a certain time is

given by the function $u(z, t)$. We also note that we can set $\Delta t = 0.5b/c$, where $c = \sqrt{G/\rho}$ is the velocity of transverse sound vibrations in the material. It can be found $u_i(z_i, t)$ for all segments at a given time if we numerically, step by step in time, solve the system of equations (1) for the initial conditions $u_i(z_i, 0) = 0$ and $\dot{u}_i(z_i, 0) = 0$ (*i.e.*, at the beginning the dislocation is straight and stationary) and the boundary conditions $u(0, t) = u(l, t) = 0$ (*i.e.*, the ends of the dislocation are fixed). This method of determining the shape of a dislocation line is called the method of discrete dislocation dynamics.

It is also possible to solve analytically the general differential equation for the same initial and boundary conditions. The general equation will be similar to Eq. (1) for a separate segment,

$$m_0 \frac{\partial^2 u(z,t)}{\partial t^2} + B \frac{\partial u(z,t)}{\partial t} - \Gamma \frac{\partial^2 u(z,t)}{\partial z^2} = f_T(z,t)\,, \tag{3}$$

and it is very easy to reduce to a standard form:

$$\ddot{u}(z,t) + 2\delta \dot{u}(z,t) - c^2 \frac{\partial^2 u(z,t)}{\partial z^2} = \frac{f_T(z,t)}{m_0}\,, \tag{4}$$

where $\delta = B/2m_0$, and $c = \sqrt{\Gamma/m_0}$ is the second definition of the velocity of transverse sound vibrations in the material. The solution of equation (4) is sought in the form of

$$u(z,t) = \sum_{n=1}^{\infty} u_n(z,t) = \sum_{n=1}^{\infty} u_n(t) \sin(\pi n z/l)\,, \tag{5}$$

where $u_n(z, t)$ is called the n-th fundamental mode of oscillations of the elastic line (in our case, the dislocation), $n = 1, 2, \ldots$ and $u_n(t)$ is a solution of the equation:

$$\ddot{u}_n(t) + 2\delta \dot{u}_n(t) + \omega_n^2 u_n(t) = f_n(t)\,, \tag{6}$$

where $\omega_n = \pi n c/l$ and

$$f_n(t) = \frac{2}{l} \int_0^l \frac{f_T(z,t)}{m_0} \sin\left(\frac{\pi n}{l} z\right) dz = \frac{2T}{m_0} \sqrt{\frac{q k_B}{l \Delta t}} Z_j\,, \tag{7}$$

where Z_j is the standard normal random variable at each time step. Further,

$$u_n(t) = \int_0^t U(t-\tau) f_n(\tau) d\tau\,, \tag{8}$$

where $U(t)$ the function satisfies the equation

$$\ddot{U}(t) + 2\delta\dot{U}(t) + \omega_n^2 U(t) = 0 \tag{9}$$

with initial conditions $U(0) = 0$ and $\dot{U}(0) = 1$. Thus,

$$U(t) = \exp(-\delta t)\frac{\exp(t\sqrt{\delta^2 - \omega_n^2}) - \exp(-t\sqrt{\delta^2 - \omega_n^2})}{2\sqrt{\delta^2 - \omega_n^2}}. \tag{10}$$

If we substitute Eqs. (7) and (10) into Eq. (8), we obtain

$$u_n(t) = \sqrt{\frac{2lk_BT}{\pi^2 n^2 \Gamma}} Z_n \left\{1 - \frac{\exp(-\delta t)}{4(\delta^2 - \omega_n^2)} \times \right.$$
$$[\omega_n^2[\exp(t\sqrt{\delta^2 - \omega_n^2}) - \exp(-t\sqrt{\delta^2 - \omega_n^2})]^2 + \tag{11}$$
$$+[\lambda_1 \exp(t\sqrt{\delta^2 - \omega_n^2}) - \lambda_2 \exp(-t\sqrt{\delta^2 - \omega_n^2})]^{1/2},$$

where $\lambda_1 = \delta + \sqrt{\delta^2 - \omega_n^2}$ and $\lambda_2 = \delta - \sqrt{\delta^2 - \omega_n^2}$, Z_n are standard normal random variables for each n. It can be seen that for a sufficiently large time t due to $\exp(-\delta t)$ formula (11) simplifies to

$$u_n(t) = \sqrt{\frac{2lk_BT}{\pi^2 n^2 \Gamma}} Z_n. \tag{12}$$

The quantity $u_n(t)$ is the amplitude of the n-th fundamental mode $u_n(z, t)$, which is a sinusoid with wavelength $2l/n$. In fact, for a sufficiently large time t, there is no explicit dependence $u_n(t)$ on t. In this case, the amplitude of the sinusoid will simply be a random variable with a normal distribution. Negative amplitude means a change in the phase of the sinusoid by π radian. It is easy to prove the correctness of formula (12), if we take into account the fact that, under thermal equilibrium conditions, the average energy of the fundamental mode of the elastic line must be equal to $k_BT/2$. The energy of the fundamental mode in our case [1] is

$$E_n = \frac{\Gamma}{2}\int_0^l \left(\frac{\partial u_n(z,t)}{\partial z}\right)^2 dz = \frac{k_BT}{l} Z_n^2 \left.\frac{2\pi nz/l + \sin(2\pi nz/l)}{4\pi n/l}\right|_0^l = \frac{k_BTZ_n^2}{2}. \tag{13}$$

The average energy will accordingly be

$$< E_n >= \left\langle \frac{k_BT}{2} Z_n^2 \right\rangle = \frac{k_BT}{2} < Z_n^2 >= \frac{k_BT}{2} \times 1 = \frac{k_BT}{2}. \tag{14}$$

Thus, the function $u(z, t)$ that determines the shape of the dislocation line under the action of random forces from the atoms in thermal motion will be a superposition of fundamental modes—sinusoids with

corresponding wavelengths and random amplitudes. If we take into account Eqs. (5) and (12), we obtain

$$u(z,t) = \sqrt{\frac{2lk_BT}{\pi^2\Gamma}} \sum_{n=1}^{\infty} \frac{Z_n}{n} \sin(\pi n z / l) . \tag{15}$$

It is important to add that, if the shape of the dislocation line is determined by the method of discrete dislocation dynamics, when the dislocation is considered as a chain $N = l/\Delta z$ of segments, then, we have $u_i(z_i, t)$ for $N+1$ points, because the left end of the dislocation corresponds to $i = 0$. We also note that, under the boundary conditions, $u_0(0, t) = u_N(l, t) = 0$. In this case, we can expand $u_i(z_i, t)$ in a series in sines:

$$u_i(z_i, t) = \sum_{n=1}^{N} A_n \sin \frac{\pi n i}{N+1} , \tag{16}$$

where

$$A_n = \frac{2}{N+1} \sum_{i=1}^{N} u_i(z_i, t) \sin \frac{\pi n i}{N+1} . \tag{17}$$

If we compare Eqs. (15) and (16), then, from their similarity, it obviously follows that

$$A_n = \sqrt{\frac{2lk_BT}{\pi^2\Gamma}} \frac{Z_n}{n} , \tag{18}$$

and variable

$$\sqrt{\frac{\pi^2\Gamma}{2lk_BT}} n A_n = Z_n \tag{19}$$

has a normal distribution with a mean value of 0 and a variance of 1. In this way, it is possible to check the correspondence of the results obtained by the method of discrete dislocation dynamics to the analytical solution of the general differential equation.

If $u_i(z_i, t)$ are calculated, then, it is possible to find the characteristics of the thermal fluctuation 'waviness' of the dislocation line, namely the standard deviation of the magnitude s_u and the average length of the section L along the axis Oz, on which $u_i(z_i, t)$ has the same sign. That is, to find the parameters, which characterize the height and length of the average convexity on the dislocation line and, thus, its critical segment. It is enough to determine simply the intersection points of the dislocation line and the axis Oz. Then, it is easy to determine the length L, which will be equal to the length of the dislocation

line l divided by the number of intersection points [34]. A feature of the definition of s_u and L are the averaging of these characteristics also over different moments of time t, *i.e.*, $u_i(z_i, t)$ should take part in the consideration not for one moment t, but for many moments.

Taking into account Eqs. (15) and (16), we can represent has a normal distribution with a mean value of 0 and a variance of 1. In this way, it is possible to check the correspondence of the results obtained by the method of discrete dislocation dynamics to the analytical solution of the general differential equation.

Taking into account Eqs. (15) and (16), we can represent

$$s_u = \sqrt{\frac{2lk_BT}{\pi^2\Gamma}}\sqrt{D\left[\sum_{n=1}^{N}\frac{Z_n}{n}\sin\left(\frac{\pi ni}{N+1}\right)\right]} = \sqrt{\frac{2lk_BT}{\pi^2\Gamma}}\bar{s}_u\,, \tag{20}$$

where $(2lk_BT/\pi^2\Gamma)^{1/2}$ contains physical quantities, $D[\ldots]$ means the variance of the random variable, which is in brackets, and in our case this quantity does not depend on any physical parameter and takes different values for different i. Numerical calculations show that $\bar{s}_u = 0.47 \pm 0.08$ for $N = 1000$. For analytical evaluation of L, a model similar to the model given in Ref. [39] can be applied. To do this, consider the distribution of positive values inside the corresponding averaged section $u(z, t)$ along the axis Oz. The length of such a section will be equal to L, by definition. If $u_i(z_i, t)$ have a normal distribution with zero mathematical expectation and standard deviation s_u, then, the sample of only positive values from them has a mean value $s_u(2/\pi)^{1/2}$. At the endpoints of such a section, $u(z, t)$ will be equal to zero, and further from each endpoint of $u(z, t)$ should increase towards the middle of the section, since the mean value of $u(z, t)$ is greater than zero. This increase will be symmetrical about the midpoint of the plot because the parts of the averaged plot on both sides of the midpoint are absolutely equal and have no advantages over each other due to the uniformity of the statistical distribution $u(z, t)$. Thus, the averaged distribution of $u(z, t)$ will be a smooth curve symmetric about the maximum at the midpoint of the plot. If we average only the positive values of the gradient $\partial u(z, t)/\partial z$ from the end point of the averaged plot to its middle, then, similarly to $u(z, t)$, we will have the average value of the gradient $s_{gu}(2/\pi)^{1/2}$, where s_{gu} is the standard deviation of the gradient. The averaged distribution $u(z, t)$ can be approximated by a suitable function, for example $A_u\cos(\pi z/L)$, where $A_u = s_u(\pi/2)^{1/2}$. Then, the average value of the gradient $\partial u(z, t)/\partial z$ on the plot, where it is positive, is $2A_u/L$, from which it is easy to obtain

$$L = \pi s_u / s_{gu}\,. \tag{21}$$

On the other hand, taking into account Eq. (15), the gradient is

equal to

$$\frac{\partial u(z,t)}{\partial z} = \sqrt{\frac{2k_BT}{\Gamma l}} \sum_{n=1}^{N} Z_n \cos\frac{\pi n i}{N+1}, \tag{22}$$

and

$$s_{gu} = \sqrt{\frac{2k_BT}{\Gamma l}} \sqrt{D\left[\sum_{n=1}^{N} Z_n \cos\left(\frac{\pi n i}{N+1}\right)\right]} = \sqrt{\frac{2k_BT}{\Gamma l}} \bar{s}_{gu}, \tag{23}$$

where numerical calculations show that $\bar{s}_{gu} = 22.36$ for $N = 1000$, that is, according to Eq. (21) for $N = 1000$,

$$L = l s_u / s_{gu} \approx l / 55. \tag{24}$$

Thus, the length L turns out to be proportional to the length of the dislocation line fixed at the ends l.

3. RESULTS AND DISCUSSION

The initial parameters for modelling the effect of thermal fluctuations on the characteristics of the average bulge on the dislocation line by the discrete dislocation dynamics method and calculating these characteristics by the analytical method are given in Table 1 [37]. The time step Δt was defined as $3.93 \cdot 10^{-14}$ s. The modelling by the discrete dislo-

TABLE 1. Initial parameters for modelling the influence of thermal fluctuations on the characteristics of the average convexity on the dislocation line [37].

G, GPa	81	m_0, kg/m	$2.5 \cdot 10^{-16}$
ν	0.3	ρ, kg/m^3	8000
α	0.123	c, m/s	3182
b, nm	0.25	Γ, N	$6.23 \cdot 10^{-10}$

TABLE 2. Temperature dependence of the drag coefficient [1].

Temperature T, K	Coefficient of motion resistance B, MPa·s
300	$3 \cdot 10^{-11}$
600	$6 \cdot 10^{-11}$
900	$9 \cdot 10^{-11}$
1200	$1.2 \cdot 10^{-10}$

cation dynamics method was carried out separately for $\Delta z = 2b$, $5b$, $10b$, $20b$ and $40b$ at a temperature of 300 K, as well as separately for temperatures of 300, 600, 900 and 1200 K at $\Delta z = 10b$. The dislocation was represented as a chain of $N = 1000$ segments. It should be noted that, under these conditions, $\Delta z = 2b$, $5b$, $10b$, $20b$ and $40b$ corresponded to the lengths of the fixed dislocation line $l = 500$ nm, 1250 nm, 2500 nm, 5000 nm and 10000 nm. The temperature dependence of the drag coefficient B is given in Table 2 [1]. During each simulation, 125000 time steps were taken, corresponding to 4.91 ns of model time. Thermal equilibrium was considered to be reliably reached after 50000 time steps, *i.e.*, after 1.96 ns of model time. The characteristics of the average bulge on the dislocation line, which were determined from the simulation results using the discrete dislocation dynamics method, were averaged for all time steps from the 50000th step to the 125000th step, *i.e.*, from 1.96 ns to 4.91 ns of model time.

An example of the dislocation line shape under the influence of thermal fluctuations, simulated by the method of discrete dislocation dynamics, at the 125000th time step ($\Delta z = 10b$, $T = 300$ K, $t = 4.91$ ns) is shown in Fig. 1. The dashed line shows the initial line shape for $t = 0$. It is seen that the dislocation line becomes randomly 'wavy' under the influence of thermal fluctuations.

The average energy of the fundamental mode (average kinetic energy of dislocation segments) from the 50000th step to the 125000th step in time, *i.e.*, in the thermal equilibrium region, is shown in Fig. 2. The discrete dislocation dynamics simulation was performed for $\Delta z = 10b$ and $T = 300$ K. The dashed line shows for comparison the standard thermodynamic value of the average kinetic energy per degree of freedom for a given temperature of 300 K $<E_n> = k_B T/2 = 0.0129$ eV.

The dependence of the standard deviation of the dislocation line points from the initial straight-line s_u on the length of this line l under the action of thermal fluctuations is shown in Fig. 3. Note that, for the simulation, $\Delta z = 2b$, $5b$, $10b$, $20b$ and $40b$ were used, *i.e.*, the lengths of the fixed dislocation line were $l = 500$ nm, 1250 nm, 2500 nm, 5000 nm and 10000 nm, respectively. The simulation was performed for a temperature of $T = 300$ K. The circles show the results of the simulation using the discrete dislocation dynamics method. The line is a calculation using formula (20), *i.e.*, an analytical method. We note a good correlation between the results of calculations using both methods. The standard deviation increases in proportion to the square root of the length of the dislocation line.

The dependence of the length L of the average bulge (critical segment) on the length of this line l under the action of thermal fluctuations is shown in Fig. 4. The simulation conditions are indicated above. The circles also show the results of the simulation using the discrete dislocation dynamics method, and the line shows the results of the cal-

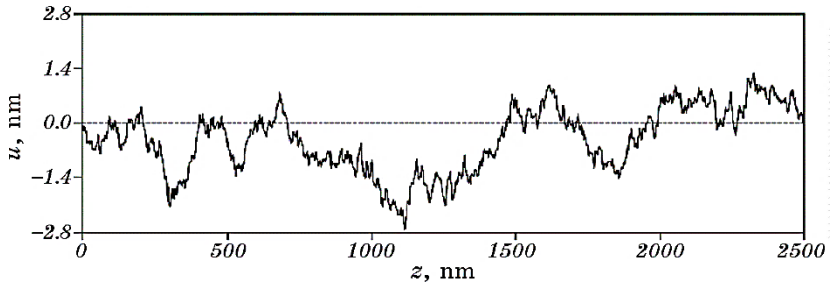


Fig. 1. Dislocation line under the influence of thermal fluctuations, simulated by the method of discrete dislocation dynamics, at the 125000th time step ($\Delta z = 10b$, $T = 300$ K, $t = 4.91$ ns); the dashed line shows the initial dislocation line for $t = 0$.

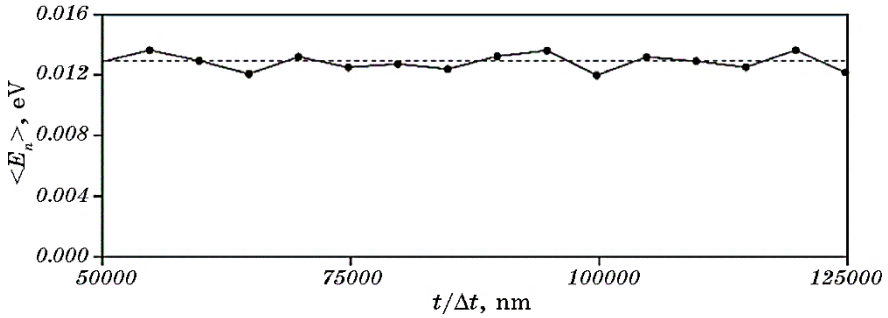


Fig. 2. The average energy of the fundamental mode (average kinetic energy of dislocation segments) from the 50000th step to the 125000th step in time ($\Delta z = 10b$, $T = 300$ K); the dashed line shows the standard thermodynamic value of the average kinetic energy per degree of freedom for a given temperature of 300 K ($k_B T/2 = 0.0129$ eV).

culation using formula (24). The results of the calculations using both methods also correlate well with each other. The length of the critical segment is directly proportional to the length of the dislocation line under these conditions.

The dependence of the standard deviation of the dislocation line points from the initial straight-line s_u on temperature at a constant dislocation line length of 2500 nm under the action of thermal fluctuations is shown in Fig. 5. Note that the simulation was performed for $\Delta z = 10b$ and temperature 300, 600, 900 and 1200 K. The circles again show the Δz results of the simulation using the discrete dislocation dynamics method, and the line is the calculation using the analytical method according to formula (20). The correlation between the results of the calculations using both methods in this case is excellent. The standard deviation turns out to be proportional to the square root of

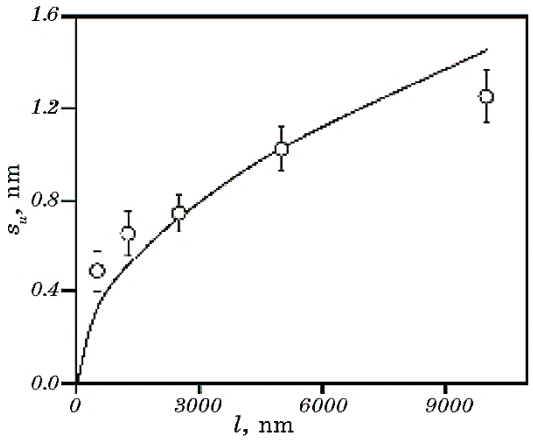


Fig. 3. Dependence of the standard deviation of the points of the dislocation line from the initial straight line on the length of this line ($\Delta z = 2b$, $5b$, $10b$, $20b$, $40b$, $T = 300$ K). Circles are calculations using the method of discrete dislocation dynamics. Lines are calculations using formula (20).

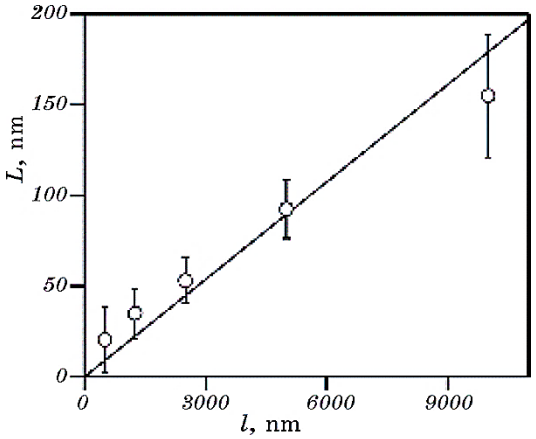


Fig. 4. Dependence of the length of the average convexity (critical segment) on the length of the dislocation line ($\Delta z = 2b$, $5b$, $10b$, $20b$, $40b$, $T = 300$ K). Circles are calculations using the method of discrete dislocation dynamics. Lines are calculations using formula (24).

the temperature.

The dependence of the length of the average bulge (critical segment) L on temperature at a constant dislocation line length of 2500 nm under the action of thermal fluctuations is shown in Fig. 6.

The simulation was performed using $\Delta z = 10b$ for temperature of 300, 600, 900 and 1200 K. The results of the simulation using the dis-

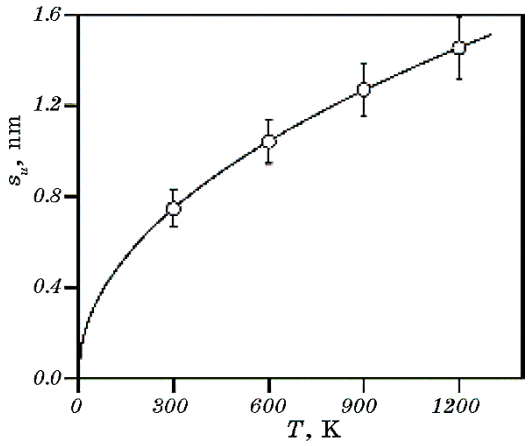


Fig. 5. Dependence of the standard deviation of the dislocation line points from the initial straight line on temperature at a constant dislocation line length of 2500 nm ($\Delta z = 10b$, $T = 300$, 600, 900, 1200 K). Circles are calculations using the method of discrete dislocation dynamics. Lines are calculations using formula (20).

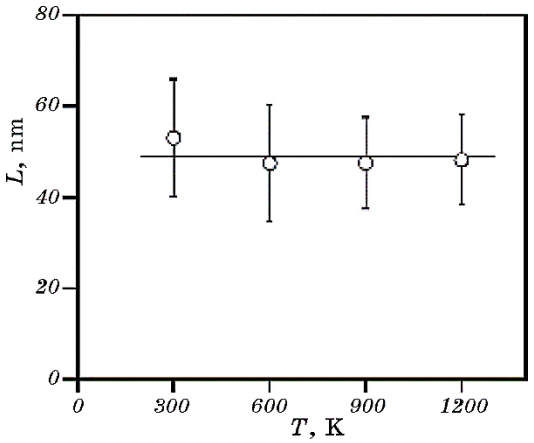


Fig. 6. Dependence of the length of the average convexity (critical segment) on temperature for a constant dislocation line length of 2500 nm ($\Delta z = 10b$, $T = 300$, 600, 900, 1200 K). Circles are calculations using the method of discrete dislocation dynamics. Line is calculations using formula (24).

crete dislocation dynamics method are shown by circles, and the results of the calculations using the analytical method (formula (24)) are shown by a solid line. The results of the calculations using both methods also confirm each other well. The length of the critical segment turns out to be independent of temperature under these conditions.

4. CONCLUSION

Thermal motion of atoms, or, in other words, thermal fluctuations or distortions of crystal lattices caused by this motion, lead to a wavy shape of the dislocation line both in alloys where there are dissolved atoms and in pure metals where there are no dissolved atoms.

The wavy shape of the dislocation line, in turn, indicates that there are obstacles to the movement of the dislocation in the material, that is, we can expect the existence of a limiting value of external mechanical stress that can initiate the movement of the dislocation, that is, the shape of the dislocation line can affect the yield point of the metal or alloy.

Thus, the characteristics of the 'waviness' of the dislocation line, namely the standard deviation of the points of the dislocation line from the straight line and the length of the averaged bulge on it under the action of thermal fluctuations, are important parameters for understanding the formation of the yield point of the material.

These characteristics, which are determined on the one hand by means of discrete dislocation dynamics and on the other hand by analytical methods, correlate well with each other, which confirms the reliability of the modelling results.

The standard deviation increases proportionally to the square root of the dislocation line length at constant temperature, and is also proportional to the square root of the temperature at constant dislocation line length.

The length of the averaged bulge, which determines the length of the critical dislocation segment, is directly proportional to the dislocation line length at constant temperature, and does not depend on the temperature at constant dislocation line length.

The determined temperature dependencies of the standard deviation of the dislocation line points from the straight line and the length of the critical dislocation segment help to understand better the effect of thermal fluctuations on the dislocation line shape.

AUTHORS' CONTRIBUTIONS

M. I. Lugovy performed numerical calculations of shear stress field in the glide plane and wrote the manuscript with input from all authors. D. G. Verbylo reviewed the literature and wrote the manuscript with input from all authors. M. P. Brodnikovskyy verified analytical approaches and provided critical feedback. T. I. Verbytska interpreted results and curated data. D. S. Leonov visualized and verified results and prepared figures/tables. M. Yu. Barabash supervised the work and devised the main conceptual ideas. All authors approved the final version of the manuscript.

REFERENCES

1. J.-H. Zhai and M. Zaiser, *Mater. Sci. Eng. A*, **740–741**: 285 (2019).
2. D. B. Miracle and O. N. Senkov, *Acta Mater.*, **122**: 448 (2017).
3. E. P. George, W. A. Curtin, and C. C. Tasan, *Acta Mater.*, **188**: 435 (2020).
4. J. D. Eshelby, *Solid State Physics*, **3**: 79 (1956).
5. R. L. Fleischer, *Acta Metallurgica*, **11**: 203 (1963).
6. R. Labusch, *Czech J. Phys.*, **31**: 165 (1981).
7. L. A. Gypen and A. Deruyttere, *J. Mater. Sci.*, **12**: 1028 (1977).
8. A. S. Argon, *Strengthening Mechanisms in Crystal Plasticity* (Oxford: Oxford University Press: 2008).
9. U. F. Kocks, A. S. Argon, and M. F. Ashby, *Prog. Mater. Sci.*, **19**: 110 (1975).
10. F. R. N. Nabarro and P. B. Hirsch, *The Physics of Metals* (Cambridge: Cambridge University Press: 1976), p. 152.
11. M. Zaiser, *Phil. Mag. A*, **82**, Iss. 15: 2869 (2002).
12. I. Toda-Caraballo, *Scripta Mater.*, **127**: 113 (2017).
13. G. P. M. Leyson, W. A. Curtin, L. G. Hector Jr., and C. F. Woodward, *Nature Mater.*, **9**: 750 (2010).
14. G. P. M. Leyson, L. G. Hector, and W. A. Curtin, *Acta Mater.*, **60**: 3873 (2012).
15. G. P. M. Leyson and W. A. Curtin, Modelling Simul. Mater. Sci. Eng., **24**: 065005 (2016).
16. C. Varvenne, A. Luque, and W. A. Curtin, *Acta Mater.*, **118**: 164 (2016).
17. C. Varvenne, G. P. M. Leyson, M. Ghazisaeidi, and W. A. Curtin, *Acta Mater.*, **124**: 660 (2017).
18. G. Laplanche, J. Bonneville, C. Varvenne, W. A. Curtin, and E. P. George, *Acta Mater.*, **143**: 257 (2018).
19. W. G. Nöhring and W. A. Curtin, *Scripta Mater.*, **168**: 119 (2019).
20. G. Bracq, M. Laurent-Brocq, C. Varvenne, L. Perrière, W. A. Curtin, J.-M. Joubert, and I. Guillot, *Acta Mater.*, **177**: 266 (2019).
21. Y. Hu, B. A. Szajewski, D. Rodney, and W. A. Curtin, *Modelling Simul. Mater. Sci. Eng.*, **28**: 015005 (2020).
22. G. Péterffy, P. D. Ispánovity, M. E. Foster, X. Zhou, and R. B. Sills, *Mater. Theory*, **4**: 6 (2020).
23. R. Pasianot and D. Farkas, *Computational Mater. Sci.*, **173**: 109366 (2020).
24. F. Otto, A. Dlouhy, C. Somsen, H. Bei, G. Eggeler, and E. P. George, *Acta Mater.*, **61**: 5743 (2013).
25. A. Gali and E. P. George, *Intermetallics*, **39**: 74 (2013).
26. S. J. Sun, Y. Z. Tian, H. R. Lin, X. G. Dong, Y. H. Wang, Z. J. Wang, and Z. F. Zhang, *J. Alloys Compd.*, **806**: 992 (2019).
27. A. V. Podolskiy, E. D. Tabachnikova, V. V. Voloschuk, V. F. Gorban, N. A. Krapivka, and S. A. Firstov, *Mater. Sci. Eng. A*, **710**: 136 (2018).
28. S. O. Firstov, T. G. Rogul, N. A. Krapivka, and S. I. Chugunova, *Metallofiz. Noveishie Tekhnol.*, **40**: 219 (2018) (in Russian).
29. S. O. Firstov and T. G. Rogul, *Metallofiz. Noveishie Tekhnol.*, **39**: 33 (2017) (in Russian).
30. S. O. Firstov and T. G. Rogul, *Metallofiz. Noveishie Tekhnol.*, **44**: 127 (2022) (in Ukrainian).
31. M. Lugovy, V. Slyunyayev, M. Brodnikovskyy, and S. O. Firstov, *Ehlektronnaya Mikroskopiya i Prochnost' Materialov*, **23**: 3 (2017) (in Ukrainian).

32. M. Lugovy, V. Slyunyayev, and M. Brodnikovskyy, *Ehlektronnaya Mikroskopiya i Prochnost' Materialov*, **25**: 26 (2019) (in Russian).
33. M. Lugovy, V. Slyunyayev, and M. Brodnikovskyy, *Prog. Natural Sci. Mater. Int.*, **31**: 95 (2021).
34. M. Lugovy, D. Verbylo, and M. Brodnikovskyy, *Uspikhy Materialoznavstva*, **2**: 19 (2021) (in Ukrainian).
35. M. Lugovy, D. Verbylo, and M. Brodnikovskyy, *Uspikhy Materialoznavstva*, **3**: 24 (2021) (in Ukrainian).
36. M. Lugovy, D. Verbylo, and M. Brodnikovskyy, *Uspikhy Materialoznavstva*, **4/5**: 12 (2022) (in Ukrainian).
37. M. Lugovy, D. Verbylo, and M. Brodnikovskyy, *Uspikhy Materialoznavstva*, **4/5**: 36 (2022) (in Ukrainian).
38. M. Lugovy, D. Verbylo, and M. Brodnikovskyy, *Uspikhy Materialoznavstva*, **6**: 15 (2023) (in Ukrainian).
39. M. Lugovy, D. Verbylo, and M. Brodnikovskyy, *Uspikhy Materialoznavstva*, **7**: 3 (2023) (in Ukrainian).
40. M. Lugovy, D. Verbylo, and M. Brodnikovskyy, *Uspikhy Materialoznavstva*, **8/9**: 13 (2024) (in Ukrainian).