occurs, which immediately relaxes by a reduction of the temperature below T_c. Hence, the strong growth of the intensity of the inelastically scattered radiation and the resulting increase of I_{TDS}/I_{Bragg} in the immediate vicinity of T_c seem to be a further hint that the phase transition is associated with the softening of an optical phonon and that at T_c a relaxational mode becomes of great importance (Wada *et al.*, 1985). Since the elastic intensity of the 0,0,10 reflection is dominated by the scattering of the Ge atoms and the contributions of both Li and O atoms are very small, the decrease in the elastic intensity in this small temperature interval around T_c indicates that immediately at the transition temperature the motion of the Ge atoms also becomes important. From the present experiments it is not possible to decide whether this decrease is caused by an increase of the Debye–Waller factor or by a displacive motion of the Ge atoms or how this behaviour is connected to the motion of the Li atoms. Since, however, in both the para- and the ferroelectric phases the equilibrium positions of the Ge atoms are nearly the same (Iwata *et al.*, 1987), a displacement seems to be less probable. The present measurements show for the first time that a lattice expansion in the *c* direction and a decrease of the elastically scattered intensity connected with an increase of the inelastically scattered intensity appears at the phase transition of LGO.

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New Aspects in the Theory of the Double Kink on a Dislocation

BY M. E. POLYAKOV

B. I. Stepanov Institute of Physics, BSSR Academy of Sciences, Leninsky prospekt 70, 220602 *Minsk, Byelorussia*

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Abstract

A theory of the double kink on a dislocation that is free of the disadvantages of previous models has been developed. In this theory the force of external action is assumed to be equal to the Peierls barrier reaction.

Introduction

As concluded by Imai & Sumino (1983), none of the reported theoretical models can explain the measured dislocation velocities. They used a high-power Röntgen generator for measurements *in situ* of dislocation mobility at elevated temperatures over a wide range of stresses in pure and doped silicon crystals. In particular, it was shown that a change of dislocation velocity with stresses for screw and 60° dislocation in highly pure crystals will be linear over the whole range of the investigated stresses and that the activation energy for the dislocation mobility does not depend on stresses.

According to Imai & Sumino (1983), the main disadvantage of previously reported experimental studies was that dislocation mobility measurements were made at elevated temperatures due to heating and cooling of a sample from room temperature to the temperatures of investigations. The distinguishing feature of the present work is that it overcomes the limitations of earlier works and makes investigations at a fixed temperature.

At the present time there are two basic theories of dislocation propagation in crystals with high Peierls barriers: the diffusion and the obstacle theories. According to the diffusion theory, a full dislocation

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velocity is determined by double-kink nucleation followed by expansion involving activation over the Peierls barriers (Hirth & Lothe, 1972). However, these authors stated that the formulas of their theory were derived intuitively. Experimental studies of the formation kinetics and evolution of excitations limiting the dislocation mobility in monocrystalline silicon have not confirmed the Hirth–Lothe model (Nikitenko, Farber & Iunin, 1987).

A significant disadvantage of the diffusion model is the use of the condition of thermal equilibrium for the kink density on dislocation (the concentration of kinks is independent of the external force). Only by ascribing the character of Brownian motion to the dislocation mobility did Kawata & Ishioka (1983) manage to bring the diffusion theory into agreement with experiment. However, such a theory cannot be true because the processes of disordered Brownian motion and ordered dislocation mobility cannot be identical.

The quantum-mechanical model of a kink on a dislocation in covalent crystals (Gosar, 1977), which represents the double kink as a quasiparticle with an elastic continuum capable of tunneling between neighboring states, has been insufficiently developed. The confirmation of the conclusions of simpler models about the thermal nature of kink diffusion can hardly be regarded as an achievement of this theory. Great hopes are pinned on the solution of the sine–Gordon equation (analog of the Frenkel–Kontorova model) for a discrete chain with a kink (Willis, El-Batanouny & Stancioff, 1986).

In obstacle theory, the dislocation mobility in semiconductors with high Peierls barriers is determined by the nucleation rate and lateral motion of the kink (Celli, Kabler, Ninomiya & Thomson, 1963; Guyot & Dorn, 1967). If external stress is absent, the dislocation will be in the valley of the Peierls relief in the position $A_0B_0C_0$ (Fig. 1). When the stress τ is applied

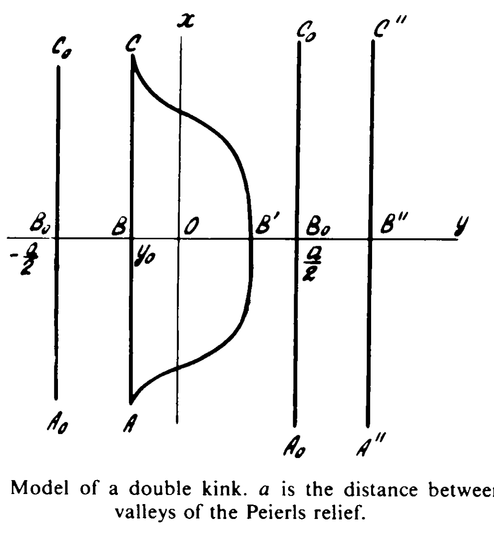

Fig. 1. Model of a double kink. a is the distance between the valleys of the Peierls relief.

in the glide plane in the direction of the Burgers vector, the dislocation is shifted to the position ABC on the slope of the barrier as shown in Fig. 1. At absolute-zero temperature, the dislocation mobility terminates at this point. In the case of elevated temperatures, the thermal fluctuations make the dislocation vibrate relative to the equilibrium position. At a sufficient value of thermal fluctuations, the dislocation loop $AB'C$ is formed, which, on attaining some critical size, will not return to its initial equilibrium position. If the loop sizes are higher than the critical ones, the two kinks involved in the loop are thought to part. As a result, the dislocation goes to the next position, $A''B''C''$, equivalent to ABC.

Calculation of the kink nucleation energy is based on the finding of the extreme energy value U for the double kink of the $AB'C$ relief from the Euler equation. The expression for U is usually written as

$$U = \int_{-\infty}^{+\infty} \{F(y)[1+(\mathrm{d}y/\mathrm{d}x)^2]^{1/2} - F(y_0) - \tau b(y-y_0)\}\,\mathrm{d}x, \qquad (1)$$

where $F(y)$ is the energy per unit length of dislocation as a function of y and b is the Burgers-vector modulus. However, analysis of this theoretical model reveals some of its serious limitations. In this model it is assumed that the energy of the applied-force action on the dislocation increases linearly with the coordinate and is not associated with the energy expended in overcoming the barrier. It also follows from the model that the force of the external action is not equal to the barrier reaction and the energy of the external action is expended even after the dislocation barrier is overcome by the segment.

The new modified model of the single kink (Polyakov, 1989) is free of the disadvantages of the previous models. The external action is equal to the barrier reaction and this ratio is reduced to the choice of proper boundary conditions, which significantly simplifies mathematical calculations. In this model the single-kink energy is

$$U = \int_{-\infty}^{+\infty} F(y)[1+(\mathrm{d}y/\mathrm{d}x)^2]^{1/2}\,\mathrm{d}x. \qquad (2)$$

From the Euler equation, one finds the shape of the kink relief on dislocation, $x = f(y)$, in the field of external forces,

$$x = (a/\pi)2^{1/2}\{[F(m)/F(0)-1]^{-1} + \sin^2(\pi y_0/a)\} \times (P^{1/2}C^{1/4})^{-1}\int_0^{\varphi} \mathrm{d}t/(1-k^2\sin^2 t)^{1/2}, \qquad (3)$$

where P, C, φ, k are the coefficients depending on the shift of the basic dislocation segment y_0 from the valley of the relief and on the ratio between the maximum $F(m)$ and the minimum $F(0)$ energy per unit of dislocation length $F(m)/F(0)$,

$$C = 1 - MN/P^2,$$
$$P = 2D\cos(2\pi y_0/a) - [1 - \cos^2(2\pi y_0/a)],$$
$$M = \sin^2(2\pi y_0/a) - 2D[1 - \cos(2\pi y_0/a)],$$
$$N = \sin^2(2\pi y_0/a) + 2D[1 + \cos(2\pi y_0/a)],$$
$$D = [F(m) + F(0)]/[F(m) - F(0)],$$
$$\varphi = \arcsin\{2C^{1/2}P/[N\tan^2(\pi y/a) + P(1 + C^{1/2})]\}^{1/2}$$
$$k^2 = (1/C^{1/2} + 1)/2.$$

On the basis of (3) the relief of the single kink in the field of external forces has been studied as a function of barrier height. It is also shown that the kink has a pseudobreak (Fig. 2). The region of the pseudobreak is characterized by a solution in the form of a meromorphic function. The dependences of the sizes of the single-kink regions and those of the pseudobreak relaxation on the barrier height and the value of dislocation shift from the relief valley (Polyakov, 1989) has been determined.

On the basis of the developed modified model of the single kink (Polyakov, 1989) it is possible to construct a model of the double kink on a dislocation and from this one may calculate the activation energy of dislocation mobility.

The modified model of the double kink on a dislocation

Since the double-kink model includes the elements of the single-kink model plus the interaction between the kinks, we can construct the double-kink model based on the modified single-kink model described by Polyakov (1989). The portions of the double kink (Fig. 3) from C' to D'' and from A' to B'' are single kinks (Polyakov, 1989). In Fig. 3, the linear portions $C'b$, dA', $B''D''$ are fixed by the external force; the portions bB', dD' are actually single kinks with relief forms (Polyakov, 1989); the portions $D'D''$ and $B'B''$ are pseudobreaks.

The minimum length of the portion $B''D''$ corresponds to the critical length of the double kink and characterizes the critical energy of the interactions between the kinks bB' and dD'. If the applied force is sustained by a constant value equal to the maximum barrier reaction (the Peierls force), the dislocation (without taking into account the dynamic losses) freely overcomes the barrier.

If the quantity of the external force is constant and its value is lower than the maximum barrier reaction, the dislocation will have the coordinate y between zero and $a/4$.

The proposed model does not use such a notion as constant stress acting on the crystal for the following reasons. Firstly, if the value of the external force is higher than the maximum quantity of the barrier reaction, the excess energy will be expended in doing work of a different kind: dislocation, acceleration and other types of energy dissipation which are not taken into account here. Further calculations use the sinusoidal Peierls barrier. This means that the force of the external action changes from zero to a maximum and back to zero with the maximum being at $y_0 = a/4$. With this approach the question arises of basic dislocation stability in the region of $a/4 < y_0 < a/2$ in which the barrier reaction reduces with increasing deviation from the stable state. In practice, the basic dislocation can reach any point y_0 in the region of $a/4 < y_0 < a/2$ with abrupt elimination of the action at the point y_0. This is possible, for example, for cyclic loading. Secondly, for a crystal both the Peierls force and Peierls stress depend on the number of dislocations in the glide plane and on the period of dislocation identity (the number of atomic planes parallel to the dislocation line in the glide plane with a nonrecurring arrangement of atoms) depending on the type of dislocation. Therefore, the value of the coordinate y_0 will hereinafter be the measure of the external effect on the dislocation.

In the previous schemes of calculation of the formation energy of double kinks, the double kink was assumed to expand under the action of the external

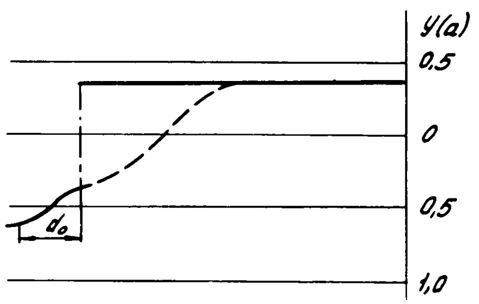

Fig. 2. Pseudobreak (the dash-dotted line) on the single kink. The dashed line represents the kink profile after pseudobreak relaxation.

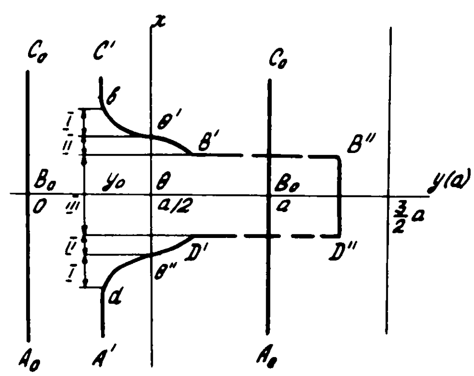

Fig. 3. A modified model of the double kink on dislocation.

force. In the proposed model, the external force moves the basic dislocation from a stable position in the relief valley to the coordinate y_0 on the relief slope and is balanced by the reaction of the primary and secondary barriers. In a two-dimensional Peierls relief, the resulting force at the point y_0 equals zero, as at all the points of kink existence. Since there is resulting force, it has no action on the lateral shift of kinks. Hence the question arises about the origin of the force balancing the interaction between the kinks.

In the model with a two-dimensional Peierls relief, the role of the frictional forces can be played by the barriers on defects (noises) and secondary barriers. In our model with a two-dimensional Peierls relief, lateral motion of the kink can only occur due to the local thermal fluctuation, unlike earlier models, in which lateral motion is performed by the same external force as migration from the valley.

If the kinks bB' and dD' collapse, the section $B''D''$ of the dislocation, for sufficient accumulated energy, can be converted into a chain of point defects, *e.g.* interstitials. Furthermore, these defects probably promote double-kink formation if they are in the glide plane. In the case where the double-kink ejection is not in the plane of dislocation migration and its subsequent collapse, the defects appear after the dislocation passage in a perfect crystal. As follows from a simplified analysis of the model, the largest number of point defects and dipoles is obtained at low stresses, high temperatures and solid loadings.

So, the present paper substantiates the model of a double kink on a dislocation that is free of the disadvantages of previous models. In the new model, the force of external action on the dislocation is equal to the reaction barrier. The external force moves the basic dislocation from its stable position in the relief valley to the y_0 coordinate on the relief slope and is counterbalanced by the barrier reaction. In a two-dimensional Peierls relief, at the point y_0 the resultant force is equal to zero as at all the points where there is a kink. Unlike the previous models in which the lateral-kink migration is caused by the same external force as the migration from the valley, in our model the lateral-kink migration is due to the thermal fluctuation over the secondary barrier. The distinguishing feature of the proposed model is the presence of a double pseudobreak on the double kink of dislocation in the field of the external force.

The presence of a break on the dislocation in no way contradicts the continuum theory of dislocation, since the break region belongs to the core of the dislocation, which is not described by the continuum theory.

In a recent study (Milchev & Mazzucchelli, 1988), a soliton break in the Frenkel-Kontorova model is mentioned. This paper analyzes an expanded Frenkel-Kontorova model with the interaction anharmonicity taken into account. Analysis of this work shows that beyond some critical value of the model parameter (displacement) there occurs a break of the discrepancy dislocation. An analytical expression for the soliton before and after the break has been obtained (Milchev & Mazzucchelli, 1988).

The formation energy of a double kink on a dislocation in nondoped crystals

Let us calculate the formation energy of a double kink for separate portions by means of a modified model. Portion I in Fig. 3 characterizes the energy required for the creation of a segment of a single kink $b\theta'$. The extreme value of the kink energy U expressed by (2) is determined by the Euler equation (Arfken, 1970)

$$(\mathrm{d}/\mathrm{d}x)\{f_0-(\mathrm{d}y/\mathrm{d}x)[\partial f_0/\partial(\mathrm{d}y/\mathrm{d}x)]\}=0, \quad (4)$$

from which, with

$$f_0=F(y)[1+(\mathrm{d}y/\mathrm{d}x)^2]^{1/2}, \quad (5)$$

we obtain

$$F(y)=C_0[1+(\mathrm{d}y/\mathrm{d}x)^2]^{1/2}. \quad (6)$$

The value of the constant C_0, obtained from the condition $\mathrm{d}y/\mathrm{d}x=0$ at $y=y_0$ and $x=+\infty$, is

$$C_0=F(y_0). \quad (7)$$

From (6) the expression for the slope of the single kink follows,

$$\mathrm{d}y/\mathrm{d}x=[F^2(y)-F^2(y_0)]^{1/2}/F(y_0). \quad (8)$$

The expression for the creation energy U_a of the single-kink segment $b\theta'$ and $d\theta''$ in the case of the barrier of a sinusoidal form

$$F(y)=F(0)+[F(m)-F(0)]\sin^2(\pi y/a) \quad (9)$$

is of the form

$$U_a=2\int_{-\infty}^{x_l}\{F(y)[1+(\mathrm{d}y/\mathrm{d}x)^2]^{1/2}-F(y_0)\}\,\mathrm{d}x. \quad (10)$$

Substituting (8) into (10) and replacing x by y, we obtain

$$U_a=2\int_{y_0}^{a/2}[F^2(y)-F^2(y_0)]^{1/2}\,\mathrm{d}y. \quad (11)$$

On numerical integration of (11) we have the dependence of the formation energy of a part of the kink on portion I on the migration depth y_0 at different ratios $F(m)/F(0)$ (Fig. 4). According to (9), the migration depth of the linear dislocation segment is proportional to the accumulated dislocation energy as a result of the external action. It is seen from Fig. 4 that the energy grows with increasing barrier height at a constant migration depth y_0 and decreases with increasing energy accumulated by the linear segment.

This dependence may be approximated by the formula

$$U_a = U(m)(a/2 - y_0). \quad (12)$$

The quantities of the formation energy of the kink on portions I, II and III make up the total formation energy of the double kink. On portion II, energy is expended in displacing the kink segment $O'B'$ from the starting point on the line $C'A'$ up to the Peierls barrier. This energy value U_a may be calculated by the formula

$$U_a = d_0[F(m) - F(y_0)], \quad (13)$$

where d_0 is the length of the single-kink region (Fig. 2) investigated by Polyakov (1989) as a function of the barrier height and y_0.

The minimum range length of portion III is determined by the energy expended in displacing the segment $B''D''$ from the position $C'A'$ up to the point θ_0 and is equal to

$$U_{r'} = r'[F(m) - F(y_0)], \quad (14)$$

where r' is the range length of the double-kink pseudobreak (Fig. 5). Equations (13) and (14) may be integrated to give

$$U_r = r[F(m) - F(y_0)], \quad (15)$$

where $r = 0'0''$. The value of r is found from the conditions of equality of two energies of which one is released at interaction of the bB'' and dD'' kinks and the other is expended in overcoming the secondary Peierls barriers or barriers on defects at kink separation.

In this paper we consider the influence of the secondary barriers because their density predominates over the density of defects. Let the secondary barrier be described by the sinusoid

$$F(x) = F'(0) + [F(m) - F'(0)] \sin^2(\pi x/c), \quad (16)$$

where $F'(0)$, $F(m)$ are the minimum and maximum energies of the length unit of the dislocation along x, respectively, and c is the period along the x axis. Let, in the first approximation, $F'(0) = F(0)_{c=a}$. Then the value of the energy $U_\delta = U_r$ expended in overcoming n secondary barriers is equal to

$$U_\delta = n[F(m) - F(y_0)](a - 2y_0), \quad (17)$$

where $x_0 = y_0$. The number n is determined from the equality condition of the energies U_δ and from the interaction of kinks Q, for which the expression for the dislocation is given in the general form (Friedel, 1956; Seeger & Schiller, 1966) as

$$Q = -[Gb^2/8\pi(1-\nu)](l^2/r) \times[(1+\nu)\cos^2\varphi + (1-2\nu)\sin^2\varphi]. \quad (18a)$$

The following designations are used: G is the shear modulus; ν is Poisson's ratio; $r = na - 2y_0$ is the distance between the kinks; $l = a$ is the barrier width and is assumed to be constant and independent of the value of external pressure from the assumption of attraction between the pseudobreaks of opposite signs; φ is an angle between the dislocation axis and the Burgers vector. In particular, for the screw dislocation, the expression for Q_s is of the form

$$Q_s = -[(1+\nu)/(1-\nu)](Gb_s^2/8\pi)(l^2/r) \quad (18b)$$

and, for 60° dislocation, Q_{60} is

$$Q_{60} = -(Gb_{60}^2/32\pi)[(4-5\nu)/(1-\nu)](l^2/r), \quad (18c)$$

where b_s, b_{60} are respectively Burgers-vector lengths for the screw and 60° dislocations. The interaction between the smooth kinks is replaced by the interaction between the sharp kinks (Fig. 5). Using (17) and (18) and taking into account the equality $F(0) = Gb^2/2$ (Nikitenko, 1975), we can write the expression for the number of secondary barriers corresponding to the critical length of the double kink on the screw

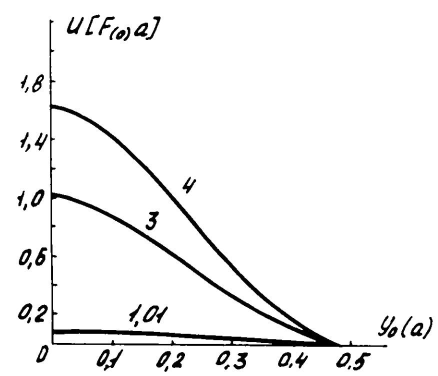

Fig. 4. The dependence of the kink formation energy in portion I on the barrier height external action force. Figures on the curves denote the $F(m)/F(0)$ ratio.

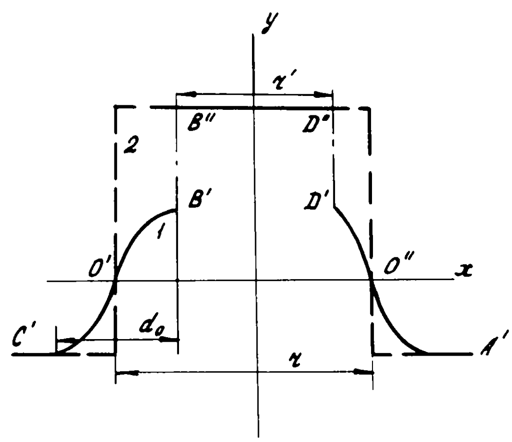

Fig. 5. An equivalent scheme for the calculation of interaction energy between the kinks: (1) the real kink location; (2) the theoretical location.

dislocation, n_s, as

$$n_s = y_0/a + \{(y_0/a)^2 + [(1+\nu)/(1-\nu)] \times [8\pi(1/2 - y_0/a)]^{-1} \times [F(m)_s/F(0)_s - 1]^{-1} \cos^{-2}(\pi y_0/a)\}^{1/2}, \tag{19a}$$

and for the 60° dislocation, n_{60}, as

$$n_{60} = y_0/a + \{(y_0/a)^2 + [(4-5\nu)/(1-\nu)]/32\pi(\tfrac{1}{2} - y_0/a) \times [F(m)_{60}/F(0)_{60} - 1]^{-1} \cos^{-2}(\pi y_0/a)\}^{1/2}, \tag{19b}$$

where $F(m)_s$, $F(0)_s$ and $F(m)_{60}$, $F(0)_{60}$ are the maximum (m) and minimum (0) energies of the screw (s) and 60° (60) dislocations.

It follows from Fig. 6 and (19a, b) that the critical length of the double kink increases monotonically with both increasing barrier width at a certain value of external action and increasing external action at a certain barrier width. However, the condition of the existence of a secondary relief is imposed on the thus calculated critical length of the double kink. For example, at $y_0 = 0.15$ (Fig. 6) the critical length of the double kink on the screw dislocation calculated by (19) is not equal to an integral number of secondary reliefs. In such cases, the steady double-kink formation is achieved if the kink covers the largest total number of secondary reliefs. If $y_0 = 0.15$, the total number of secondary reliefs characterizing the steady state of the double kink is 6. The reasonable critical length of the double kink as a function of y_0 is marked in Fig. 6 by a step curve. At certain y_0 the energy $U_\delta(s)$ expended in overcoming the n_s secondary barriers corresponding to the critical length of the kink on the screw dislocation can be determined from (17),

$$U_\delta(s) = 2n_s F(0)_s a[F(m)_s/F(0)_s - 1] \times (\tfrac{1}{2} - y_0/a)\cos^2(\pi y_0/a), \tag{20a}$$

where

$n = 5$, $0 < y_0 < 0.105a$,

$n = 6$, $0.105a < y_0 < 0.17a$,

$n = 7$, $0.17a < y_0 < 0.21a$,

⋮ ⋮

and $U_\delta(60)$ for the 60° dislocation is

$$U_\delta(60) = 2n_{60}F(0)_{60}a[F(m)_{60}/F(0)_{60} - 1] \times (\tfrac{1}{2} - y_0/a)\cos^2(\pi y_0/a) \tag{20b}$$

at

$n = 3$, $0 < y_0 < 0.065a$,

$n = 4$, $0.065a < y_0 < 0.18a$,

$n = 5$, $0.18a < y_0 < 0.245a$,

⋮ ⋮

Then the expression for the energy of double-kink (dk) formation on the screw dislocation, $U_{dk}(s)$, may be written as

$$U_{dk}(s) = U_a(s) + U_\delta(s) = 2\int_{y_0}^{a/2} [F^2(y)_s - F^2(y_0)_s]^{1/2}\,dx + 2n_s F(0)_s a[F(m)_s/F(0)_s - 1] \times (\tfrac{1}{2} - y_0/a)\cos^2(\pi y_0/a). \tag{21a}$$

$U_{dk}(60)$ for the 60° dislocation is

$$U_{dk}(60) = U_a(60) + U_\delta(60) = 2\int_{y_0}^{a/2} [F^2(y)_{60} - F^2(y_0)_{60}]^{1/2}\,dx + 2n_{60}F(0)_{60}a[F(m)_{60}/F(0)_{60} - 1] \times (\tfrac{1}{2} - y_0/a)\cos^2(\pi y_0/a) \tag{21b}$$

and U_{mgr} is the energy of kink migration over the secondary barrier, equal to U_δ at $n = 1$ and y_0.

It may be seen from Fig. 7 that the values of the energies of double-kink formation for both screw and 60° dislocations decrease unevenly with increasing external action. Thus it is noted that an important feature of the new model of a double kink on dislocation is the uneven drop of the double-kink formation energy depending on the monotonic increase of the external force action for both 60° and screw

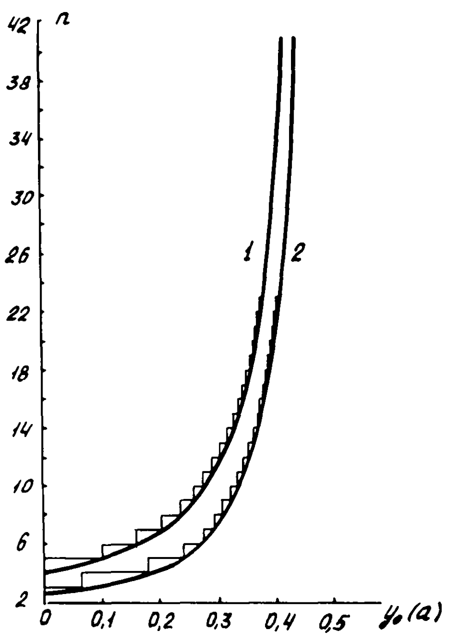

Fig. 6. The critical length of the double kink on screw (1) and 60° (2) dislocations at $F(m)/F(0) = 1.01$.

dislocations. This fact is attributed to the presence of a secondary Peierls relief.

From the new model of a double kink an analytical expression has been obtained for the double-kink formation energy depending on the critical double-kink length, the value of dislocation migration from the Peierls relief valley and the Peierls energy.

Concluding remarks

A model of a double kink on dislocation that is free of the disadvantages of the previous models has been substantiated. The distinguishing feature of the proposed model is the presence of a double pseudobreak on a double kink on dislocation in the external force field.

A feature of the new model is the uneven decrease in the double-kink formation energy depending on the monotonic increase of the external action for both 60° and screw dislocations. This is due to the periodicity of the secondary Peierls relief.

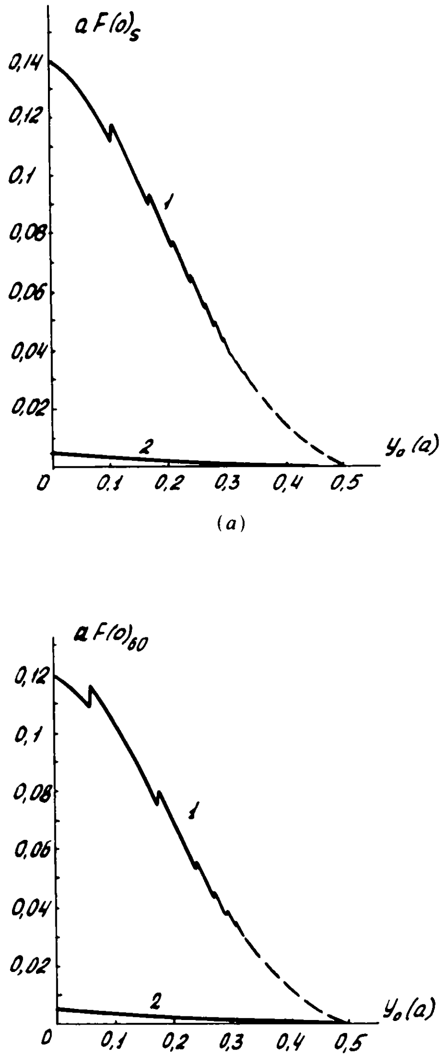

Fig. 7. The activation energy of double-kink formation U_{dk} (curve 1) and kink migration U_{mgr} (curve 2) of (*a*) screw and (*b*) 60° dislocation *versus* the external force at $F(m)/F(0) = 1.01$.

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