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Analysis of the Motion of Frenkel-Kontorova Dislocations in Single Crystals of Aluminum with Allowance for the Peierls Barrier

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Abstract

The regularities of the motion of a one-dimensional Frenkel-Kontorova dislocation in pure aluminum at helium temperatures are studied. Computer simulation was carried out using the sine Gordon equation, written in dimensionless variables. It is proven that when the transition to dimensionless variables the discreteness of the model is preserved. The dependence of the true values of stresses on deformation in the Euler variables, as well as the velocity distribution of the dislocation fragments along the coordinate for successive instants of time, are obtained. It is shown that under these conditions dislocation motion is realized by quantum tunneling of the dislocation bends. The quantum-mechanical estimate confirms the possibility of quantum tunneling of the kink of dislocations in aluminum at low temperatures.

Subject Areas

Mechanics, Modern Physics

Keywords

Aluminum, Frenkel-Kontorova Dislocation, Sine Gordon Equation, Computer Simulation, Dislocation Kinks, Quantum Tunneling

1. Introduction

Many elements of modern technology operate under conditions of moderate (up to 200 K) and deep (up to 4 K) cooling. These are elements of liquefaction and separation plants, spacecraft systems, etc. It was found that with decreasing temperature most of the metals become more durable. At 77 K (the boiling point of liquid nitrogen), the strength of copper is doubled, and the strength of alu-

minum is six times larger than at room temperature. At low temperatures, especially under load, internal structural transformations occur, which increases the risk of sudden destruction of products. The transition of metals into a fragile state at low temperatures is associated with a change in the plasticity characteristics. Investigations of the physical nature of the problem show that the transition to the fragile state of pure single crystal samples depends on temperature, rate of deformation, dislocation density, etc.

Although a large number of studies are being carried out in this direction, for example [1] [2], the developed physical models do not allow to quantify the influence of numerous factors. A number of questions remain unclear, in particular, the problem of an abnormal decrease in the plastic flow stress in aluminum at low temperatures.

Therefore, a study of the nature of the change in the strength and plasticity parameters of metals as a function of temperature and deformation rate at temperatures from 293 K to the boiling point of liquid helium (4.2 K) is of great scientific interest.

2. Theoretical Background

In the plastic region, unlike the elastic region, qualitatively new physical phenomena are realized. If a volume change occurs in the elastic region with a change in the stress state, then the physics of the phenomenon changes radically in the region of plasticity. Dislocations move under the condition that the volume is constant, and the dependence of the yield stress on the accumulated deformation has a nonlinear character. For most deformable metals, the transition from elasticity to the plasticity region is of a smooth nature, so a 0.2% residual deformation is considered as the conditional boundary of such a transition, and the corresponding stress is called the conditional yield point. Therefore, in the region of plasticity, conditions for the constancy of volume are used to obtain the stress-strain relation [3]. For sufficiently large plastic deformations, to compare the results of the theory with experiment, the conditional values of stresses and deformations go to their real values.

In [4] the nonlinear dependence of the yield stress on the accumulated deformation, strain rate and temperature is

$$\sigma = a_0 \varepsilon^{a_1} \zeta^{a_2} \exp^{-a_3 \theta} \tag{1}$$

where $a_0 = 3.6 \times 10^6$ MPa, $a_1 = 0.255$, $a_2 = 0.05$, $a_3 = -0.01$, a_0, a_1, a_2, a_3 -constants of material, ζ -rate of deformation, θ -temperature on Celsius scale.

In the case of a dislocation description of the plasticity of single crystals, the kinks on dislocations are the carriers of the mass, they start to slide at a force much less than that required for dislocation motion as a whole. In this case, a linear dislocation can be represented as an elastic string lying initially in one of the local minima of the potential. The smallness of the effective mass and the large inflection mobility at low temperatures ($T < 50$ K) [5] suggest the possibility of tunneling such a quasiparticle through the Peierls barriers and then pulling

the remaining part of the dislocation there.

It follows from the deformation diagram [3] that, beginning with the strength limit of the material, when the deformation increases, its localization takes place, the active stress increases intensively and the sample breaks down. However, if a sharp decrease in the true stress occurs at stresses below the true value of the tensile strength, the interpretation of this result requires additional assumptions.

The simulation was carried out using sine Gordon equation for the one-dimensional Frenkel-Kontorova dislocation model. In the Frenkel-Kontorova model, the atoms above the glide plane are material points connected by springs of rigidity «*k*», and the atoms under the glide plane (substrate) are described by a sinusoidal potential. The Frenkel-Kontorova model is discrete and this is its advantage over other models. Within the framework of the chosen model, the motion of dislocations is described by the sine Gordon equation.

$$m\ddot{y}_n = -f_0 \sin\left(2\pi y_n / a\right) + k\left(y_{n+1} + y_{n-1} - 2y_n\right) \tag{2}$$

where y_n is deviation of the n-th atom from the equilibrium position, a -lattice constant, $f_0 \sin\left(2\pi y_n / a\right)$ -periodic sinusoidal force on the substrate side, *m*-mass of the atom, *k*-stiffness coefficient.

In dimensionless units, the sine Gordon equation takes the form:

$$\ddot{\varphi}_n + \sin\varphi_n - \varphi_n'' = 0 \tag{3}$$

where φ_n is displacement n-th atom from the equilibrium position.

When changing to dimensionless variables, finite differences are replaced by spatial derivatives. However, the discreteness of the model is preserved. We will carry out the corresponding analysis. The dislocation size is determined as follows [6]:

$$l_0 = a\sqrt{mv_0^2 / 2\pi f_0 a}$$

$v_0 = a\sqrt{k/m}$ -speed of sound, l_0-size of dislocation, *a*-inter-atomic distance. The denominator is the product of the force at a distance, which is obviously proportional to the work that must be spent on overcoming the Peierls barrier separating one valley from the other. Thus, it increases with increasing spring stiffness and decreasing forces on the substrate side. Assuming that the elastic energy greatly exceeds the work, we obtain that $l_0 \gg a$. It follows from the condition obtained that we are considering the case of the long-wave approximation. Using the sine Gordon Equation (3), we model the displacement field, the deformation field, and the stress field near the dislocation.

As can be seen from the numerical experiment, the strain field is discrete, it decreases to the right and to the left of the dislocation line and, oscillating, tends to zero away from the dislocation line. The oscillations are obviously due to the barriers of Peierls, since in pure metals at low temperatures they are the main obstacle to the motion of dislocations. As can be seen from **Figure 1(b)**, there are no finite solutions in the region of the dislocation core, which is in agreement with [6].

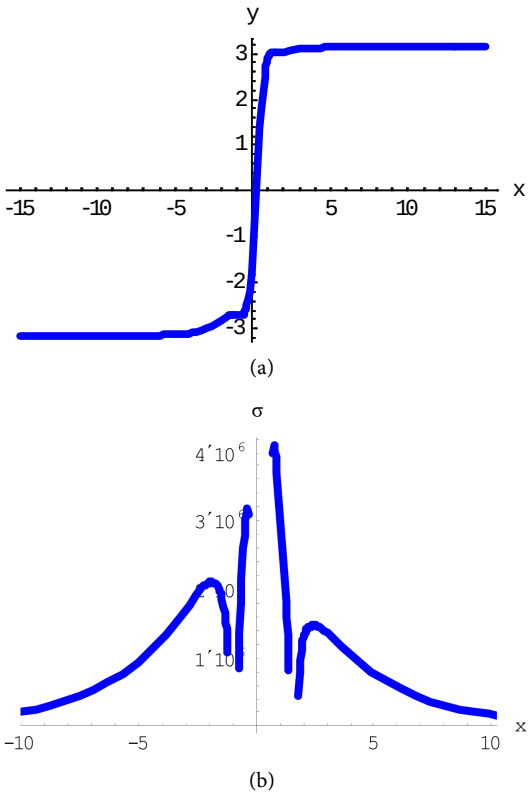

Figure 1. The displacement field of the dislocation (a) and the stress field around the dislocation (b).

In particular cases, the sine Gordon equation admits the solution in an analytical form. In more complex cases, approximate solutions of the inhomogeneous sine Gordon equation are obtained using perturbation theory (e.g. [7]). We investigate solutions of the inhomogeneous sine Gordon equation in numerical form.

The initial conditions were taken by us, using a known analytical solution of the homogeneous sine Gordon equation at the initial instant of time. The simplest boundary conditions, which have a physical meaning, consist in the fact that the sample through which the dislocation propagates is considered open at both ends,

$$\partial\varphi/\partial x\big|_{x=0} = \partial\varphi/\partial x\big|_{x=l} = 0$$

where l-dimensionless sample length.

There are two equivalent approaches when considering the motion of a deformable material: the Euler approach and the Lagrange approach. When attention is concentrated on a given point in space into which different particles of a deformed medium come, this is the Eulerian approach. Movement from the Eulerian point of view is known if speed, acceleration, temperature, etc. are given as functions of coordinates of a given point of space and time-these are Euler variables. When attention is concentrated on a particular particle of the medium and the history of its deformation and motion is studied, this is the Lagrange

approach. The choice of the kind of variables is made on the basis of the nature of the problem to be solved. We solve the problem using Euler's approach.

The problem was solved by us in the Eulerian analysis for the following reasons. Under the Eulerian approach, we study the characteristics of the change in the field of a moving dislocation at a given point in space over time. In the Lagrange case, the evolution of the motion in the space of a given point of the dislocation field is investigated.

The nonlinear differential sine Gordon equation, with which we describe the motion of dislocations, is also used in the description of weak superconductivity in the Josephson tunnel junction between two closely located superconductors. In addition, for certain values of the parameters it goes over into the Klein-Gordon equation, which is a quantum equation. Therefore, we assumed that the phenomenon of tunneling of inflections can be described by a sine Gordon's equation.

3. Results. Discussion

By numerically solving the sine Gordon Equation (3), using the initial and boundary conditions given above, we get the dependence $\varphi_n(x,t)$. Next, from the displacement function, we go to deformations, then using the experimentally obtained (describing the true stresses and deformations) dependence of mechanical stress on deformation, deformation rate and temperature (1), we find the dependence of the true stresses on deformation in aluminum at helium temperatures in Euler variables **Figure 3(a)**.

As is known, the conditional tensile strength for aluminum is 8×10^8 dyne/cm^2.

Using a known relationship between true and conditional stresses $\sigma_{tru} = \sigma_{con}(1+\varepsilon)$ [3], for the true value of the tensile strength, we obtain the value $8\times10^8(1+\varepsilon)$ dyne/cm^2, where ε-the coordinate of the abscissa at the beginning of the descent. If the values of σ_n, at which the curve starts to go down $\sigma_n < 8\times10^8(1+\varepsilon)$, then the tunneling effect occurs, if at any of these points the value σ_n is greater than the true value of the tensile strength, then deformation is localized and the sample is destroyed.

From the data of the numerical experiment (**Figure 3(a)**) we calculated the true values of stresses and deformations at which a sharp softening occurs (the descents on the curve), and compared the obtained values of the stresses at these points with the true value of the aluminum tensile strength (**Table 1**).

As a result, we can conclude that in our numerical experiment at points of sharp softening (points (1-6) in **Figure 3(a)**), the crystal fracture cannot happen, the stress values at these points are less than the true value of the tensile strength. It follows from the numerical experiment (**Figure 3(b)**) that the velocity of dislocation movement relative to the medium is periodic.

In the interval of decrease in the dislocation velocity, hardening takes place, the decrease in the dislocation velocity is due to an increase in the resistance of

Table 1. True values of stresses and deformations at which a sharp softening occurs and the true value of the tensile strength.

	ε	σ	$8 \times 10^8 (1 + \varepsilon)$
1	0.185	2.73×10^6	9.48×10^8
2	0.254	2.94×10^6	10.032×10^8
3	0.267	3.06×10^6	10.136×10^8
4	0.288	3.1×10^6	10.304×10^8
5	0.358	3.26×10^6	10.864×10^8
6	0.465	3.42×10^6	11.72×10^8

the medium from the side of the Peierls barrier. The consequence of this is an increase in stress. When the dislocation falls into the valley of the potential Peierls relief, the resistance to movement of the dislocation decreases sharply, as a result of which the stress is relaxed (softening) and the sign of the dislocation velocity reverses. Thus, when the Peierls barrier is overcome, the dislocation moves, slowing down before the barrier and accelerating after overcoming the barrier (3b), *i.e.* processes of micro-hardening and micro-softening occur periodically. Consequently, the nature of the stress variation in the vicinity of the investigated region (near the dislocation) reflects the above-mentioned character of the dislocation motion (**Figure 3(c)**), caused by the discrete nature of the medium: the softening has an almost periodic character.

We assume that a sharp decrease in the stress with an almost constant deformation, which is periodic in nature, can be explained by tunneling of kinks through the Peierls potentials.

From this point of view, the result presented in **Figure 3(a)** can be explained as follows. When a dislocation moves, a stress field is created around it, that reflects the nature of the evolution of the medium properties. When the Peierls barrier is overcome, the dislocation moves jump wise, slowing down before the Peierls barrier and accelerating after overcoming the barrier (**Figure 4**). Because of this, the nature of the stress variation in the vicinity of the investigated region (near the dislocation) reflects the above-mentioned dislocation movement pattern, caused by the discreteness of the medium: softening (tunneling) has a periodic character, which correlates with the oscillating dependence of the deformation on the coordinate (**Figure 2(b)** and **Figure 2(c)**), the growth of the curve $\sigma(\varepsilon)$ is nonlinear.

As can be seen from **Figure 3** and **Figure 4**, the tunneling process, as expected, is non stationary.

It is seen from **Figure 4** that the velocity of individual fragments of dislocation (kinks) during tunneling is different and changes sign during the slip, the dislocation moves waveringly, oscillates in the direction of sliding. The result obtained agrees with the results of [8], where it is shown that at low temperatures in copper and aluminum deformation acquires an abrupt nature. The experimentally observed low-temperature jump-like deformation in aluminum is also described in the review [9].

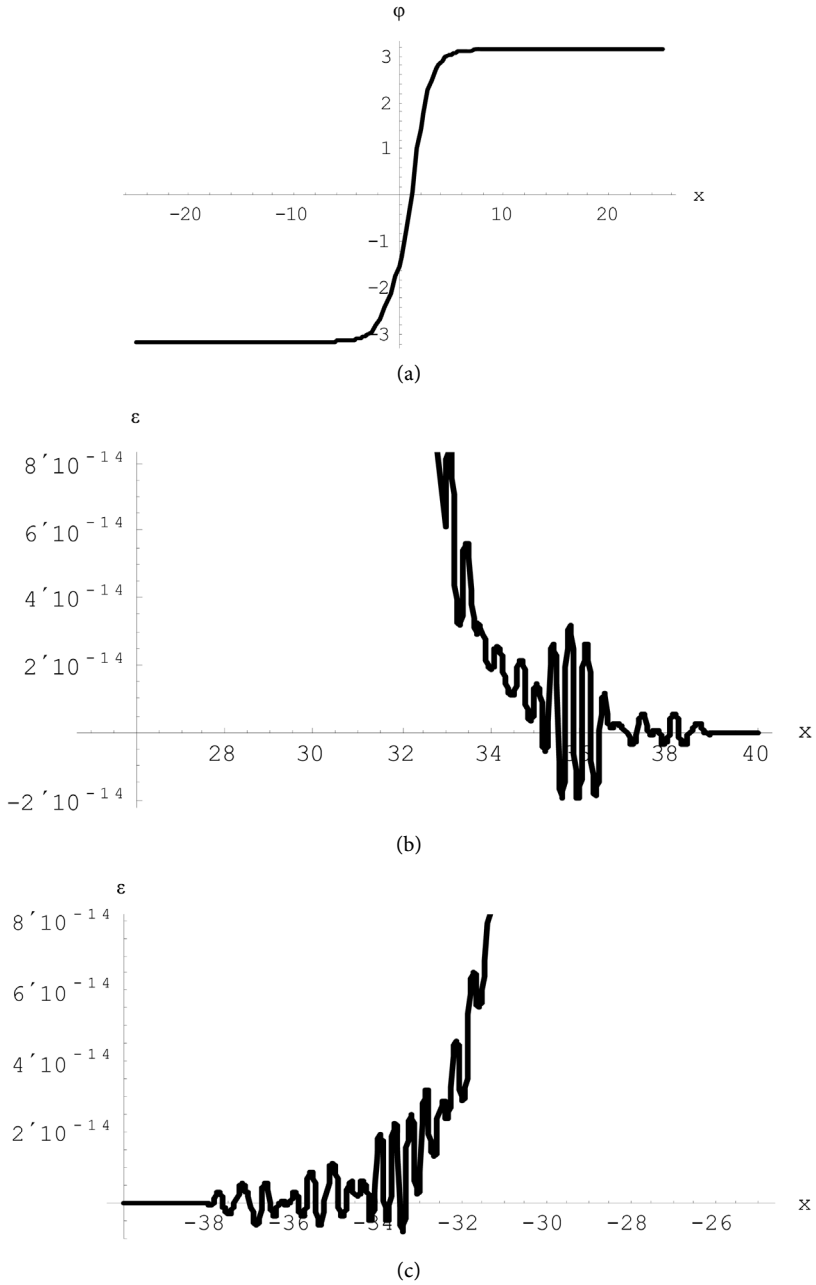

Figure 2. The dislocation displacement field (a), the deformation field to the right of the dislocation (b), the deformation field to the left of the dislocation (c).

It is known that in aluminum at low temperatures an abnormally high creep rate is observed, which in the literature [10] [11] is interpreted on the basis of quantum-mechanical models. In metals at low temperatures dislocation motion is ensured by moving relatively small distances of a large number of small-scale fragments. In aluminum samples, only the kinks of dislocations can be noticeable mobility, which can be regarded as point defects (quasiparticles) on dislocations. It is known from quantum mechanics that the tunneling condition for a quasiparticle through a potential barrier has the form $\frac{2}{\hbar}\sqrt{2m_s\left(W_p - E_{ks}\right)}l \approx 1$

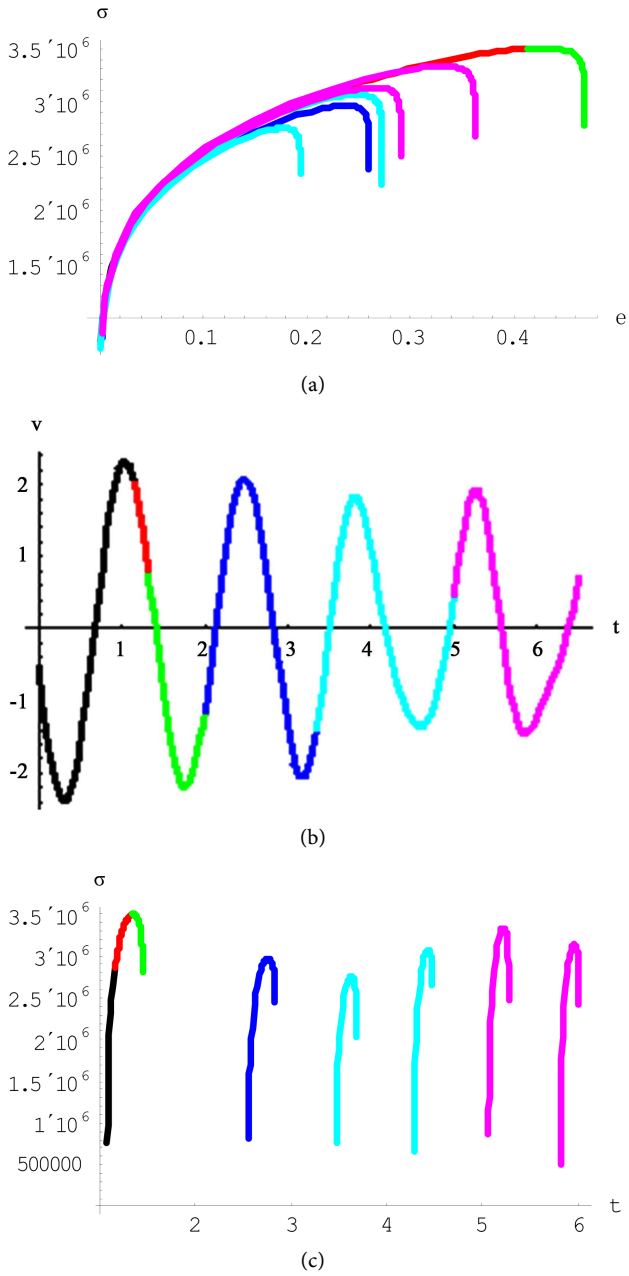

Figure 3. (a) The stress-strain dependencein the Euler variables; (b) Dependence of dislocation velocity on time for the same time intervals; (c) The dependence of the stress on time in the vicinity of the dislocation for the same time intervals.

($\hbar$-Planck's constant, m_s-effective kink mass). Calculations give that for kinks in aluminum $\frac{2}{\hbar}\sqrt{2m_s\left(W_p - E_{ks}\right)}l \approx 0.73$, which confirms the possibility of tunneling of kinks.

Quantum effects in crystals are observed when the wave functions of atoms in neighboring sites overlap. The probability of quantum tunneling of an atom into an adjacent lattice site is characterized by the dimensionless de Boer parameter [12]:

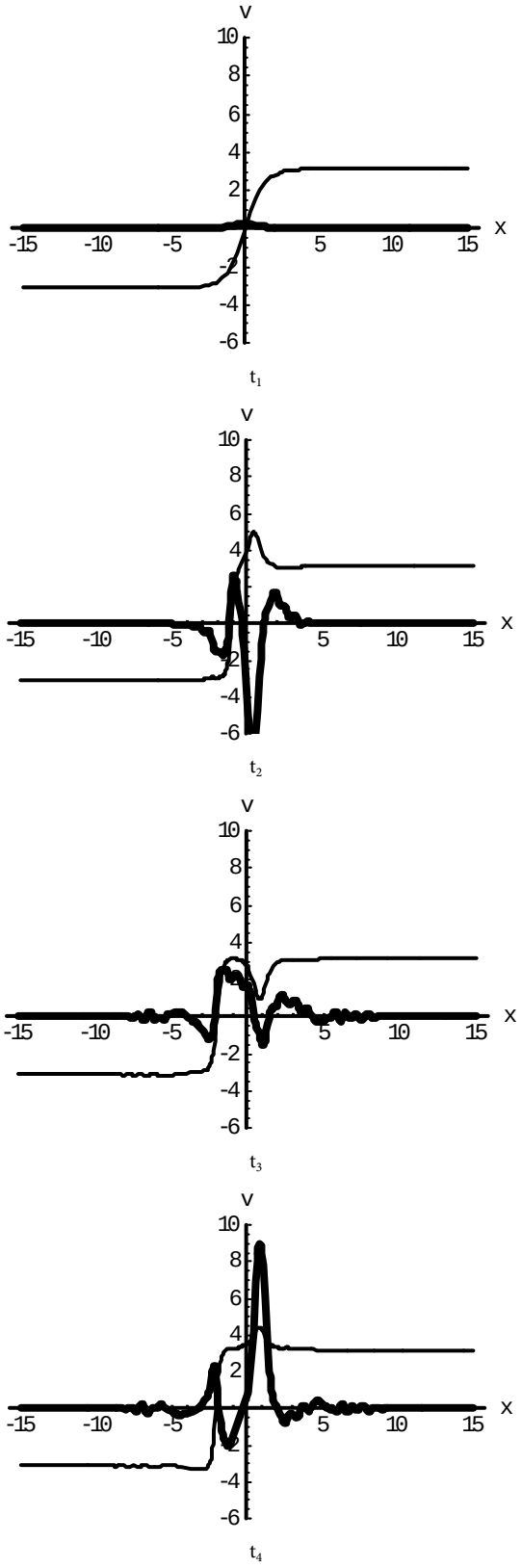

Figure 4. The displacement field of a dislocation moving by way of kinks tunneling, and the coordinate distribution of velocities of the same dislocation (a bold line) for successive instants of time.

$$\Delta \sim \frac{h}{a}(mu)^{1/2}$$

where a is the inter atomic distance, m is the mass of atoms, and u is the energy of interaction of neighboring atoms. For most crystals the parameter Δ is very small. In quantum crystals $\Delta \sim 1$ and the delocalization effect of particles is significant. Because of the smallness of the mass of the kinks and their weak interaction with the matrix atoms, the kink can be delocalized in the crystal, while the atoms of the matrix themselves behave in a classical way.

Calculations show that in aluminum, $u \sim 10^{-14}$ erg and $\Delta \approx 0.4$ (for comparison, in quantum crystals for He^3, $\Delta \approx 0.49$, for neon $\Delta \approx 0.07$. In all pure metals the parameter Δ is negligibly small [12]).

The result obtained speaks in favor of the fact that tunneling is possible.

4. Conclusion

Thus, numerical modeling, theoretical estimation and comparison with experiment allow us to conclude that in pure aluminum (99.9998%) at low temperatures (4.2 K) the anomalously high creep rate can be explained by quantum tunneling of the dislocation kinks.

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