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New Atomic Model of Metals Plastic Deformation

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Citation

Abstract

Nowadays, many aspects of physics of strength and plasticity are explained from the view point of dislocation theory. In an article a new discrete model of plastic deformation is submitted for consideration which is based on the idea of instability. Depending on the form of the interatomic interaction a potential crystal lattice can be stable or be in the state of unstable equilibrium. The crystal lattice is at the state of unstable equilibrium in solids with the spherically symmetric potential of interatomic interaction. These solids are plastic and they are mostly metals. The crystal lattice can change its state under the influence of external conditions – pressure and temperature. On the two-dimensional model of the crystal it is shown that the state of unstable equilibrium is caused by the displacement of atoms from the position with minimum potential energy. The crystal lattice looses its stability under the influence of low external stress and it results the atomic planes shear. The atoms move to the position with lower potential energy. The mechanism of the crystal lattice transition into the state of unstable equilibrium is described. The experimental data are given, thus confirming the proposed new discrete model of plasticity of solids.

1. Introduction

Modern physics of strength and plasticity is based on the strong belief that metals with perfect crystal lattice should be high strength. This means that for the shear of atomic planes in the crystal lattice of the ideal structure extremely high shear stress is need. The basis for such views is the high values of the modules of metals elasticity.

However, for real metals and their alloys the resistance to shear is by two three orders of magnitude lower than theoretically calculated. For eliminating contradiction between these theoretical and experimental data the dislocation model has been created. It is assumed that the presence small number of dislocations in real crystals decreases shear resistance to atomic planes slipping. This point of view on the nature of plasticity of metals was offered by Taylor, Orowan and Polanyi in the 1930s. Now the dislocation model is the basis of physics of strength and plasticity. In the past, the dislocation model was not recognized by many scientists. Nevertheless, the critical attitude has not prevented from spreading it, because the best model of the metals plasticity has not been offered up to now.

The most simple and obvious is the model of an edge dislocation (figure 1a). The edge dislocation is a linear defect that occurs in the area of incomplete atomic planes of the crystal lattice. The presence of the edge dislocation in the crystal implies the availability of nearby atoms, which are significantly displaced from their equilibrium. In general dislocation is a combination of atoms, which moved on the crest of the potential barrier

(figure 1b). This provides the displacement of the atomic planes of the crystal under the influence of relatively
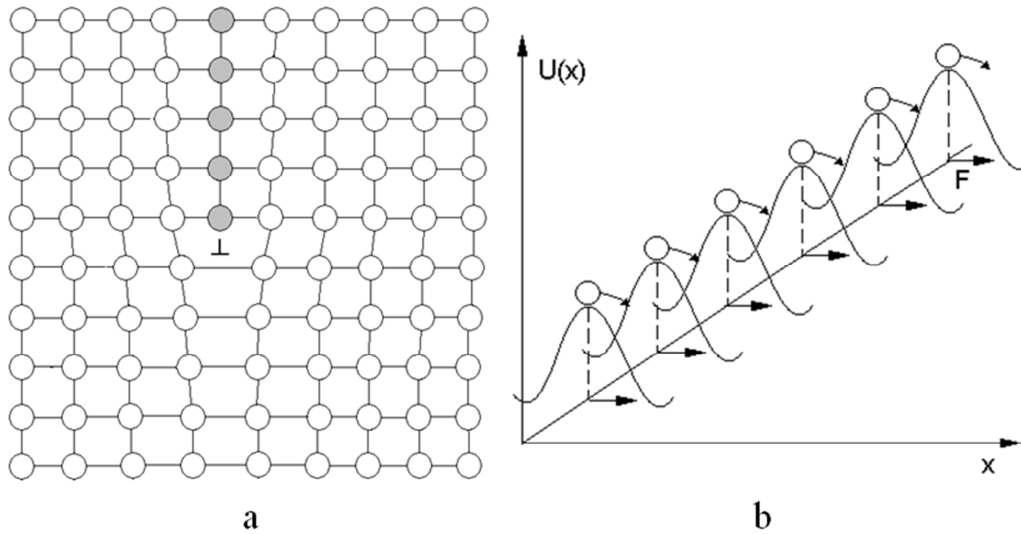
insignificant external stresses [1].

Figure 1. An edge dislocation (a), in which the atoms are displaced from the position with minimum potential energy (b) [1].

Thus, the presence of dislocations in the crystal transforms its local area into the state of unstable equilibrium. Under small external force the atoms move to the position with minimum potential energy (figure 1b). Therefore, the process of plastic deformation of solids should be considered as the loss of crystal lattice stability relatively to shear strain under the action of external forces [1-10].

Using the edge dislocation only one elementary act of plastic deformation can be explained – shear of the atomic planes on one interatomic distance. For further shear of atomic planes generation of new edge dislocations are needed. In addition, for explanation of all aspects of plastic deformation, except edge dislocations, other complex models of dislocations are used: screw, twinning, grain-boundary, helicoidal, mixed, partial, vertex, prism, pair, complete, stretched, partial Franc's, Lamer-Cottrell's dislocations, disclination. Also different additional of models are used: dislocations creep, annihilation, generation (source the Frank-Rid) and other. In explaining of metals strength there is dualism. For example, high strength of metals is explained both by the presence of a small number of dislocations and also by the presence of large numbers of dislocations [11-14]. Thus, the explanation of the phenomena of plasticity in using the dislocation model is complex and difficult for understanding and in some cases is contradictory.

In this regard, the article suggests for considering a new model that explains the plastic deformation on the atomic level.

In the new model the existence of dislocations in solids is not denied. Their presence, generation and movement during plastic deformation were confirmed experimentally. These results are undeniable. In general, they also were not denied by the opponents [11, 15, 16] of the dislocations theory. Moreover, they admitted that during the process of crystallization in real crystals both distortions of the «nonius" type can be generated and curving of the screw type dislocations. However, they objected to the fact that the dislocations have the special property of mobility and that it distinguishes them substantially from all other lattice defects. On the contrary, in their opinion, dislocations are not directly related to the occurrence of plastic deformation and that they are not substantially different from all other lattice defects [13].

The basis of the new suggested model like the dislocation one is that the crystal lattice's atoms are at an unstable equilibrium state. The difference between two models is that in the dislocation model being in the state of unstable equilibrium the atoms are just in the local regions of the crystal lattice. In the proposed model, all the atoms are in the state of unstable equilibrium, except the surface atoms. Therefore, the ability to plastic deformation is one of the basic properties of the ideal crystal lattice of metals, while according to dislocation theory, the crystals which does not contain dislocations, does not display plastic properties. Note that the provisions of the proposed model coincide with the early views on the plasticity of metals of Y. I. Frenkel, A. V. Stepanov, T. A. Kontorova, M. B. Klassen-Neklyudova and other [11, 15, 16].

2. Theoretical Method

Previously [9, 10] on a two-dimensional lattice it was shown that under high temperature (near the temperature of crystallising) a stable crystal lattice was formed in which the atoms are placed in the position of minimum potential energy (figure 2, curve 3). In such crystal lattice for shear of the atomic planes substantially expenditure of energy is required. But, due to the decreasing temperature, the atoms are displaced from the position with low potential energy to the position with a little bit higher potential energy. In this case,

under displacement of atom together with the atomic plane in the crystallographic direction [100] (figure 2, curves 1 and 2) its energy decreases. These results are confirmation of the fact that with decreasing temperature the crystal lattice transforms into the unstable equilibrium state.

It should be also noted that for atom displacement in the direction [110] the considerable expenditure of energy is needed (figure 2, curve 4).
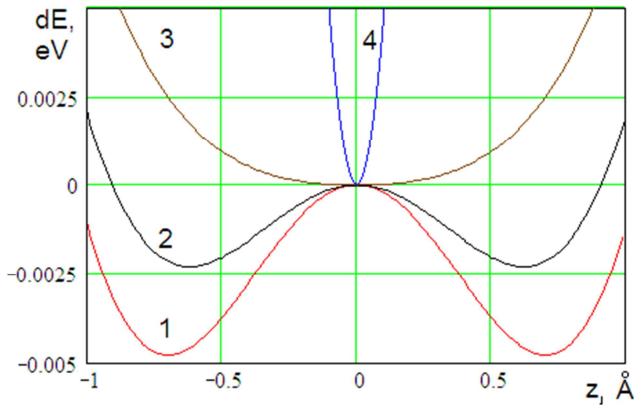

Figure 2. *The change of a potential energy dE, when an atom shifts with a plane in the direction [100] - 1, and in the direction of [110] - 4 at different temperatures: 1,4 - T_1; 2 - T_2; 3 – T_3, $T_3 > T_2 > T_1$.*

The decreasing of the temperature is only one of the reasons of the crystal lattice transition into the state of unstable equilibrium [8]. A special question which requiring additional explanation is the mechanism or way of the transition of the crystal lattice into the state of unstable equilibrium. Below will examine this in more detail.

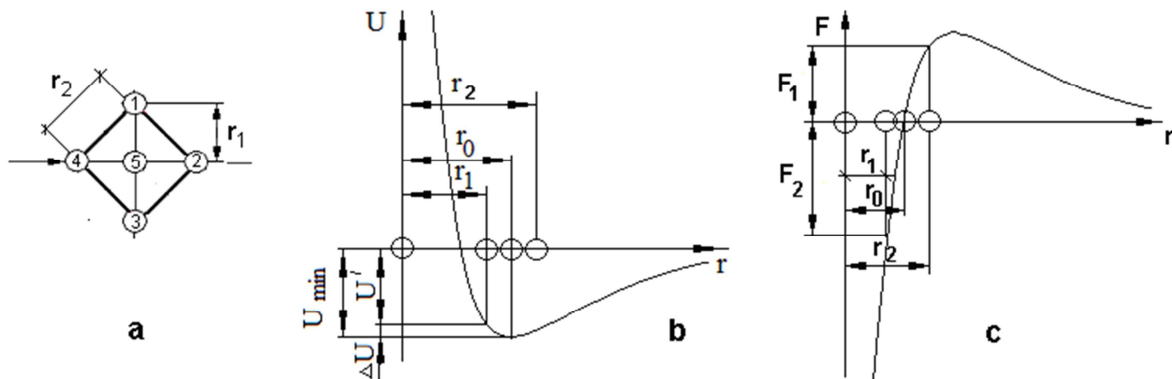In the general case the formation of the particular crystal lattice depends on the nature of interatomic interaction, which in turn depends from the electron density distribution of valence electrons in space.

If the electron density distribution of the valence electrons is spherically symmetric, the forces of interaction $F = f(r)$ is only the function of the distance r and the bond is non-directional. Each atom tends to surround itself the greatest possible number of neighbours – this is a case of ionic and metallic bonds.

If this distribution is anisotropic, then in spherical coordinates the force of the interatomic interaction will be $F = f(r,\varphi,\theta)$, where φ,θ are spatial angles, and connections are directed. The number of nearest atoms's neighbours (the coordination number) is equal to the number of directions in which electron density is maximum. This is a case of covalent bonds [14].

Since we are talking about plastic materials, let's consider the first case – the interaction of atoms with spherically symmetric potential in pentatomic model of the crystal (figure 3a).

3. Results and Discussion

3.1. The Transition of the Crystal Lattice into the State of Unstable Equilibrium

In Figure 4a given the results of calculation of the potential energy of the pentatomic crystal *Ek* depending on the interatomic distance *r*, are obtained according well-known methodology [9, 10, 14]. The potential energy of the crystal determined as the sum of the potential energies of all the atoms of the crystal. The potential energy of atoms calculated as the sum of the energies of the pair interaction of the atom with its neighbors.

Figure 3. *A pentatomic model of the crystal (a). The dependence of energy U (b) and force F (c) of interaction between atoms at diatomic model from the distance r.*

In Figure 4b given the potential energy *E* of the atom 5 depending on the interatomic distance *r* between atom 5 and its four neighbors interacting with atom 5.

The crystal is in equilibrium when its potential energy is minimum. The position of minimum potential energy in the graph (figure 4a) determines minimum of the distance of the crystal, which is equal to r_1 = 2,34 Å. In this case, the distance between the closest atoms is less than the equilibrium distance $r_1 < r_0$, where r_0 =2.5 Å is the equilibrium distance (figure 3b). Therefore, the crystal lattice is compressed. Through that between central atom 5 and peripheral atoms 1, 2, 3, 4 the repulsive forces F_2 will be acting (figure 3c). The repulsive forces F_2 are balanced by attraction forces F_1, which occur between the peripheral atoms because the distance between them is greater than the equilibrium distance - $r_2 > r_0$.
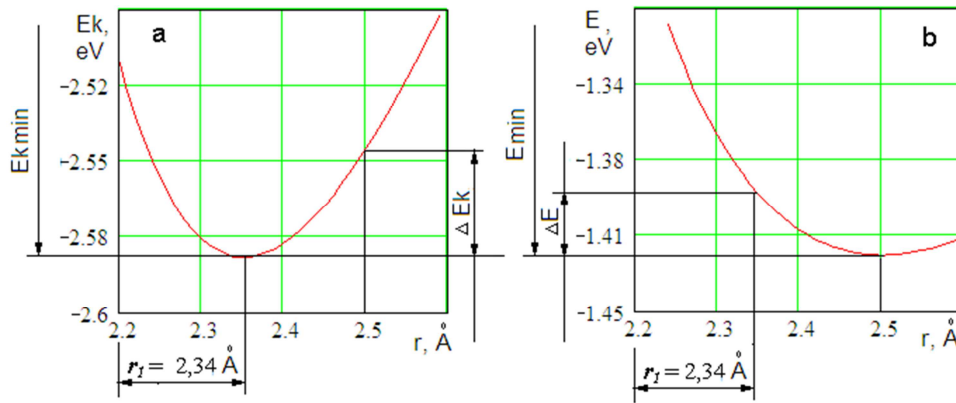
Figure 4. *The dependence of the potential energy E_k of the crystal (a) and dependence of the potential energy E of the atom 5 at diatomic model (b) on the distance r between atoms.*

Due to the distance between atoms of pentatomic model is decreases the potential energy of the atom 5 is increases by ΔE (figure 3b and 4b). This placement of atoms in the crystal corresponds to absolute zero temperature. With increasing the temperature the distance will increase between atom 5 and its neighbors to a distance of $r_1 = r_0 = 2.5$ Å. The energy of atom 5 will decrease to ΔE and will be minimum (figure 3a and 4b).

Thus at high temperature (after crystallization) the crystal is stable but at temperatures decreasing it transforms into a state of unstable equilibrium, since the potential energy of atom 5 is above the minimum. This conclusion is true for large crystals too. The stable state of their internal atoms transforms at the state of unstable equilibrium when a temperature decreases.

Under the action of external force, atom 5 moves to a new position together with atoms 4 and 2. In this case the potential energy of atoms 4 and 5 decreases (figure 5) but for atom 2 will increase.

Therefore, for the displacement of the atomic planes in the crystal energy expenditure is needed.

Overall, the amount of energy which is needed for the shear at the pentatomic crystal is the difference between the energy required to shear the surface atom 2 and the energy released during the displacement of atoms 4 and 5. It is obvious that with increasing number of the atoms in the crystal cross section of an energy loss for the shear of the atomic planes is decreased.

Figure 5. *A two-dimensional crystal: a - unstable equilibrium; b – the crystal after deformation.*

Consequently, a transition to the a state of unstable equilibrium of the crystal lattice occurs due to the displacement of atoms to positions that, do not meet their minimum potential energy. It occurs because the crystal lattice compression due to the temperature decreasing and spherical symmetric potential of interatomic interaction.

3.2. The Crystal Lattice in the State of Stable Equilibrium

Let's consider the second case when the distribution of the electron density of the valence electrons is anisotropic. Then the interatomic bonds are directed. In such solids the crystal lattice is at the state of stable equilibrium. Because of it the displacement of the atomic planes can only occur under high stress. Such solids have high strength and they are not plastic. But under the influence of high hydrostatic pressure it could be converted into plastic. Additional a rapprochement of atoms increases potential energy, and causes a transition of the crystal lattice in the state of unstable equilibrium. This is confirmed by studies [17] of high hydrostatic pressure effects on the energy change of an atom in the case of displacement of atomic planes in a two-dimensional crystal lattice with an asymmetric potential of the interatomic interaction (figure 6).

According to the obtained graphs (figure 6b), in the case of displacement of atom 1 together with the atomic plane in the direction [100] (curve 1), the potential energy increases when the high hydrostatic pressure is absent. In the case of the action of high hydrostatic pressure the potential energy decreases (figure 4b, curve 2 and 3), which means the loss of stability and transfer of the crystal lattice into the unstable equilibrium state.

It is known that all solids, regardless of the type of chemical bonds, under the action of high hydrostatic pressure become plastic and become conductive. The reason for this is the additional rapprochement of atoms. Due to the rapprochement of atoms a zone of valence electrons overlaps with a zone conduction, that is, the collectivization of valence electrons is happened.
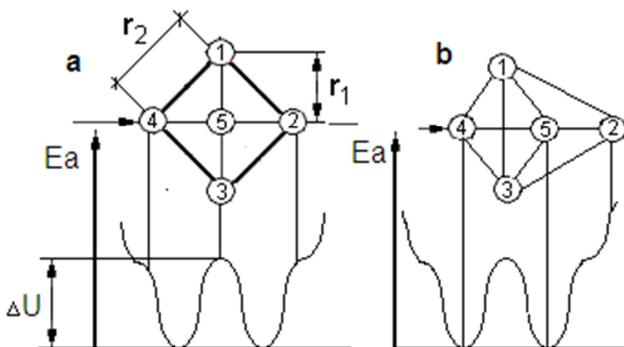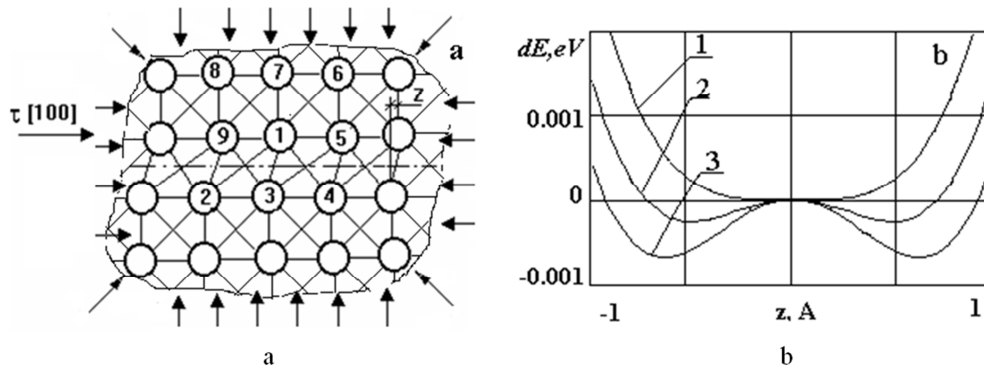
Figure 6. The displacement of atomic planes under the action of pressure (a); the changing of energy under displacement of atom 1 with the atomic plane (b) in the direction [100] at normal conditions - curve 1- P_1 and under the action of hydrostatic pressure - curves 2 - P_2 and 3 - P_3. $P_3 > P_2 > P_1$.

On the other hand, the further rapprochement of atoms their potential energy is increased, and that is cause a transition a crystal lattice at a state of unstable equilibrium. For metals the electrical conductivity and ductility are characteristic under normal conditions. For metals these properties are typical at normal conditions. Therefore, that fact confirms that a crystal lattice of metals is compressed due to the specifics interatomic interaction, as mentioned above.

Thus, at metals the decreasing distance between the atoms is due to the internal forces, and at not plastic solid bodies under external forces. In both cases, the process of plastic deformation is a consequence of the loss of stability of the crystal lattice under the action of shear stresses. The atoms move to the position with minimum potential energy.

3.3. Experimental Confirmation of the Proposed Model

According to the proposed model, the ideal crystal lattice which to be at the state of unstable equilibrium, should have low shear strength and should be high plasticity. Experimental data on the investigation of the strength of bulk metal single crystals of high purity and perfect structure are proof of that [11, 18-22]. These single crystals have extremely low shear resistance. A number of researchers who investigated their mechanical properties argue that in such crystals in general may not have the shear resistance. For example: 191 p., [18]. "The crystal begins to flow under the influence of such a low force that even to date remains an open question whether there is in the case of perfect crystal of pure metal is any strict boundary elastic stretching" c.23 [22]." A plastic flow in metallic single crystals occurs for any small stresses. This means that the actual limit of elasticity (yield stress) for these crystals is zero."

Thus, a metal single crystals of high purity and perfect structure are highly plastic and low strength that is consistent with the conclusions of the proposed model. High strength polycrystalline metals are due to the presence boundaries of grains and blocks, and various defects, including dislocations.

Experimental confirmation of the theory of dislocations is very high strength of thin crystals - 'whiskers'. Their strength

is by one to two orders of magnitude higher than the strength of technical metals and their alloys [23, 24]. It is believed that this high strength is due to the perfect structure of a crystal lattice "whiskers". But "whiskers" have a surface that is a defect. It is well known [22, 25-27] the structure of the surface layers different from the structure of a perfect crystal lattice. The ideal structure of a crystal lattice is possible if the number of atoms is infinity.

In the case of a limited number of atoms, the ideal structure will occupy only a part of the volume of the crystal. In the surface layers the atoms are arranged differently and have different properties. Therefore, the surface is a specific type of plane defect and has a significant influence on the physical-mechanical properties of metals, namely, an elastic stage of deformation, the limit of proportionality and yield stress, the overall shape of the curve "stress-strain" and the various stages of strain hardening; on the processes of fatigue and fracture, creeping and recrystallization [22].

A significant influence of the surface results in a high strength of small diameter crystals, less than 5 μm (figure 7). With the increase of the diameter of the whiskers the effect of the surface decreases and the strength decreases. If the size of crystals is greater than 50 μm, their strength is comparable with the strength of real metals [23, 24]. In big metallic single crystals the influence of the surface mostly disappears and its strength is close to zero, as mentioned above.

Thus, high strength whiskers cannot be the experimental proof of the initial postulates of the theory of dislocations.
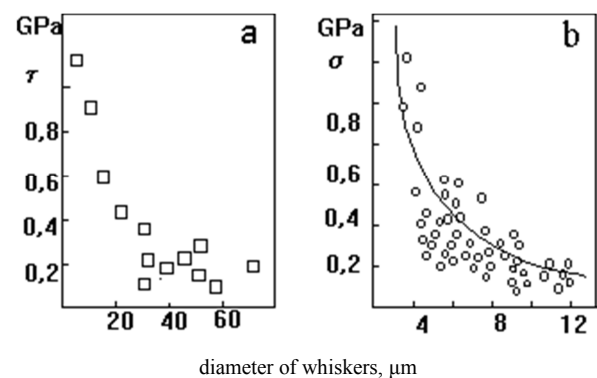

diameter of whiskers, μm

Figure 7. Stress of shear - a [23] and yield strength b [24] for iron whiskers in dependence from the crystals size.

4. Conclusion

Depending on the nature of the electron density distribution of the valence electrons the geometry of the interatomic interaction potential is formed. Atoms with a spherically symmetric potential of interaction mostly creates a crystal lattice that is in a state of unstable equilibrium. Atoms with an asymmetric potential creates a stable crystal lattice.

Plasticity and strength of solids with a perfect crystal lattice depend on its state. Solids with the crystal lattice which is in the state of unstable equilibrium are plastic and not strong. They are mainly metals and their alloys. Solids with the crystal lattice which is in the state of stable equilibrium are high strength and brittle.

Plastic deformation is the simultaneous displacement of the atoms from the position of unstable equilibrium in to a stable position in an ideal crystal lattice. In this case, the resistance to shear is absent or negligible, if the displacement of the atomic planes occurs along the crystallographic directions the most thickly strung with atoms (crystallographically preferred).

The presence of defects in real metals (surface layers, boundaries of blocks and grains, dislocations, vacancies and on) increases the resistance to shear of atomic planes and make it stronger.

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