Electronic structure of solids and their plastic properties

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ABSTRACT

This article examines the relationship between the electronic structure and the mechanical properties of solids. It is shown that these properties depend on the spatial distribution of valence electron density—whether it is isotropic or anisotropic. This distribution determines the geometry of the interatomic interaction potential. In the case of an anisotropic distribution, an asymmetric potential with directional bonding is formed. Solids with such an interatomic interaction potential possess a stable crystal lattice. Conversely, when the valence electron distribution is isotropic, a spherically symmetric interatomic interaction potential is formed. In this case, the crystal lattice of solids becomes unstable under shear deformations. The cause of this instability is self-compression, which arises due to the spherically symmetric nature of the interatomic interaction potential. The plasticity and strength of solids depend on the state of the crystal lattice. Solids with a stable crystal lattice are strong and non-plastic, whereas those with an unstable lattice are plastic and lack strength. A plasticity model of the crystal is proposed, in which the unstable crystal lattice is stabilized by a surface layer whose properties and structure differ from those of the inner layers. The resistance to shear of atomic planes in such a crystal is primarily determined by the surface layer. The magnitude of this resistance depends on the crystal size: in small crystals, the resistance to atomic plane displacement is high, approaching the theoretical limit. In large crystals, this resistance is comparable to the shear resistance in a crystal model with an edge dislocation. The presence of internal defects further increases crystal strength.

I. INTRODUCTION

In modern materials science, defects in the crystal lattice are considered to play a crucial role in determining the mechanical properties of solids, particularly strength and plasticity. These properties are considered dependent on the structural characteristics of solids, with little emphasis on their relationship with electronic structure. However, the tendency of certain materials to undergo plastic deformation depends not only on the presence of specific defects—such as dislocations—but also on their electronic structure, particularly the type of chemical bonding.[1–6]

Among all crystalline solids, metals exhibit the highest plasticity. In contrast, most crystalline materials with covalent and ionic bonds are low-plastic and brittle. It is important to note that the type of bonding is the primary factor determining the plasticity of solids, while structural factors play a secondary role. Dislocations are present in ionic, covalent, and metallic crystals, yet only metals

exhibit high plasticity. Moreover, among all crystalline solids, metals are also the best conductors of electric current. The connection between the electronic structure and the mechanical properties of solids is particularly evident in the relationship between electrical conductivity and plasticity. This connection was previously explored, albeit unsuccessfully, by Frenkel.

He observed that metals, especially single crystals, exhibit high plasticity and electrical conductivity prior to mechanical processing, whereas dielectrics are non-conductive and brittle, particularly at low temperatures. Consequently, he concluded that the high plasticity of metals is related to the presence of collectivized electrons, although the nature and origin of this connection remained unclear.[4]

The relationship between the electronic structure of solids and their mechanical properties—strength and plasticity—has been examined within the configurational model of matter developed by

Samsonov and his collaborators.[5] According to this model, in the condensed state, two subsystems of valence electrons can coexist—partially localized and collectivized—which determine the strength and plasticity of materials.

Arkharov and his colleagues,[6] building on this model, concluded that in metals, regions with a high degree of valence electron delocalization (regions with a well-structured crystal lattice) coexist with regions where valence electrons are more localized (defective areas of the material), which are characterized by covalent bonding. Accordingly, a metal contains both more plastic and less plastic regions.

The conclusions of Samsonov and Arkharov regarding the relationship between electrical conductivity and plasticity in metals are largely credible. However, similar to Frenkel, they did not provide an explanation for the underlying reasons behind this connection. The origin of the coexistence of two subsystems of valence electrons remains unclear. Additionally, the effects of external parameters, such as temperature and pressure, on these phenomena were not addressed.

Consequently, the study of the relationship between the electronic structure and the mechanical properties of solids remains a highly relevant area of research today.

II. INFLUENCE OF ELECTRONIC STRUCTURE ON THE MECHANICAL PROPERTIES OF SOLIDS

The mechanical properties of solids, such as plasticity and strength, depend on their electronic structure, particularly on the spatial distribution of valence electron density.[7,8] Two types of distributions are possible: isotropic and anisotropic (Fig. 1). Depending on the nature of the valence electron density distribution, the geometry of the interatomic potential can take one of two forms:

- A spherically symmetric potential.
- An asymmetric potential.

In the case of an isotropic electron density distribution, a spherically symmetric interatomic potential is formed. Under such
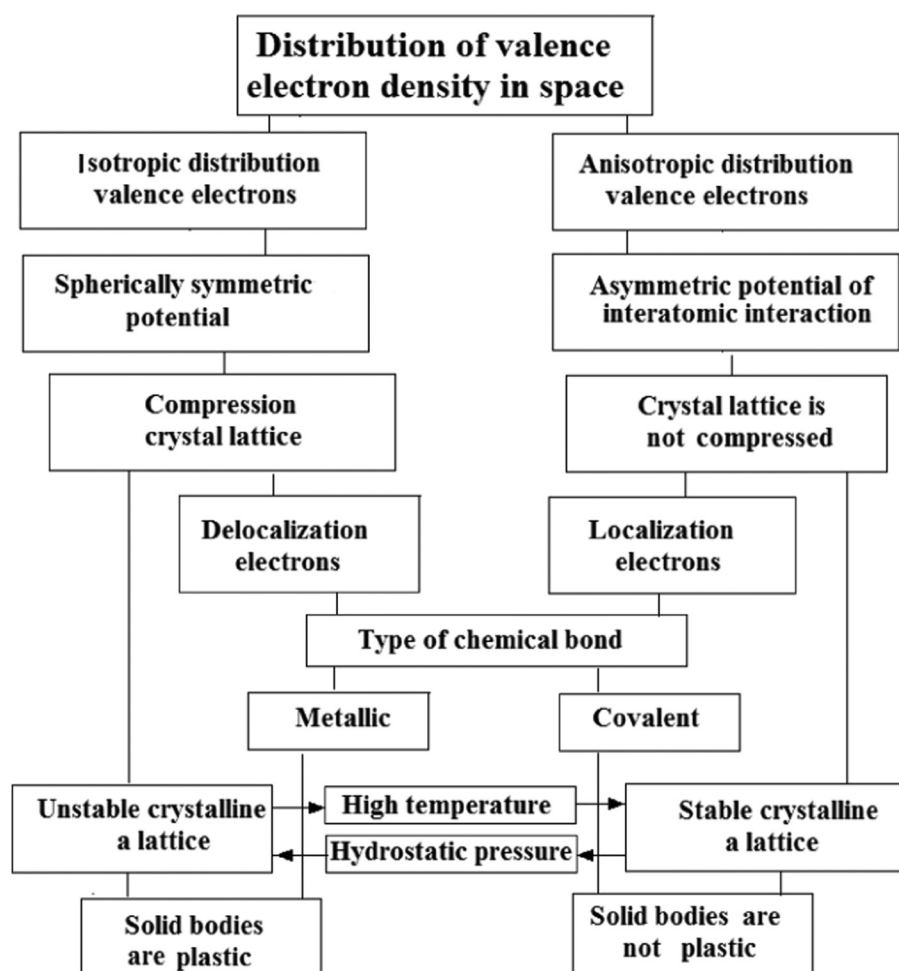

FIG. 1. Electronic structure and mechanical properties of solids.

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a potential, the force F depends only on distance, $F = f(r)$, leading to non-directional bonds. This type of interaction is characteristic of metallic bonding. In contrast, when the valence electron density distribution is anisotropic [in spherical coordinates, $F = f(r, \phi, \theta)$], the bonds become directional, which is typical of covalent bonding.[7,8]

Solids with covalent bonds exhibit high strength. They are characterized by low electrical conductivity and plasticity, or, in many cases, a complete lack of plasticity. In contrast, metals are both plastic and electrically conductive.

For a spherically symmetric interatomic potential, the crystal lattice of solids (primarily metals) undergoes self-compression.[9–11] Due to compression, the potential energy of atoms is not at a minimum. As a result, the lattice becomes unstable, which induces its plasticity. More details on the causes of self-compression are provided below.

Self-compression of the crystal lattice results in additional atomic displacements, leading to the overlap of the valence and conduction bands. This overlap causes the delocalization of the electron gas, resulting in high electrical conductivity. In general, self-compression of the crystal lattice leads to high plasticity and electrical conductivity in metals, similar to how high hydrostatic pressure induces these properties in non-metallic solids.

However, in the case of an anisotropic distribution of valence electron density, the interatomic potential is asymmetric and directional, which is characteristic of a covalent bond. In this case, crystal lattice compression is absent, leading to the formation of a stable crystal structure. Such solids have low plasticity and electrical conductivity or may lack these properties entirely. They are typically semiconductors or dielectrics.

Environmental parameters—pressure and temperature—have a significant influence on the stability of the crystal lattice. Under their effect, the interatomic distance changes. A decrease in interatomic distance under high hydrostatic pressure increases plasticity and electrical conductivity, whereas an increase in interatomic distance at high temperatures reduces these properties.

It is worth noting that this article does not consider the effect of pressure and temperature on changes in electronic configuration, which can lead to polymorphic transformations.

III. SELF-COMPRESSION OF THE CRYSTAL LATTICE IN METALS

Theoretical and experimental data[12–16] indicate that all solid bodies, under the influence of high hydrostatic pressure, acquire metallic properties, namely, electrical conductivity and plasticity. The additional rapprochement of atoms due to external forces is the main reason for the transformation of solid bodies into plastic and electrically conductive materials, meaning they develop metallic bonding. In the absence of external forces, they lose these properties. Thus, under high hydrostatic pressure, all solid bodies exhibit metallic properties.

Given the high plasticity of metals, it has been hypothesized that internal forces exist within them, compressing the crystal lattice. The assumption that the crystal lattice of metals is compressed has been confirmed through theoretical studies of two-dimensional models using molecular mechanics methods.[17] These studies have shown that in the case of a spherically symmetric long-range interatomic potential [see Fig. 2(b)], the crystal lattice is indeed compressed.[9–11]

The reason for this compression lies in the fact that, under such a potential, attractive forces act between distant atoms in the unit cell [see Fig. 2(a)]—specifically, atoms 1, 2, 3, and 4. These attractive forces are counterbalanced by repulsive forces between the nearest atoms (1–5, 2–5, 3–5, 4–5) [Fig. 2(c)]. As a result, the unit cell undergoes compression, and the distance between the nearest atoms, r_1, becomes smaller than the equilibrium distance, r_0, i.e., $r_1 < r_0$.

Previous research studies[18–20] have reported cases of additional atomic rapprochement to distances shorter than the equilibrium distance under normal conditions.

IV. INSTABILITY OF THE CRYSTAL LATTICE

The self-compression of the crystal lattice in metals is crucial for understanding the relationship between electrical conductivity and plasticity. As a result of compression, atoms move closer together, leading to the overlap of the valence band with the
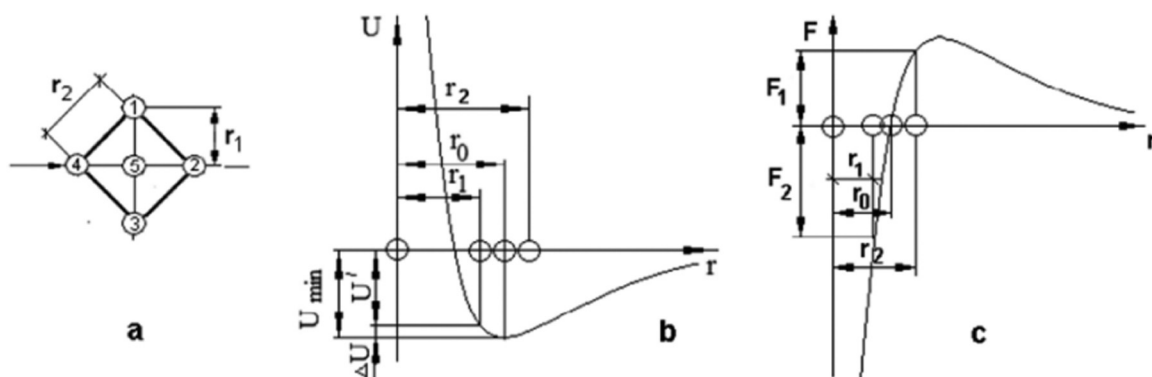
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FIG. 2. A pentatomic model of the crystal (a). The dependence of energy U (b) and force F (c) of interaction between atoms in a diatomic model on the distance r.[11] Adapted from L. Kozak, AASCIT J. Mater. **3**(5), 26–32 (2017). Copyright 2017 Association of Asian Scientific Journals for Material.
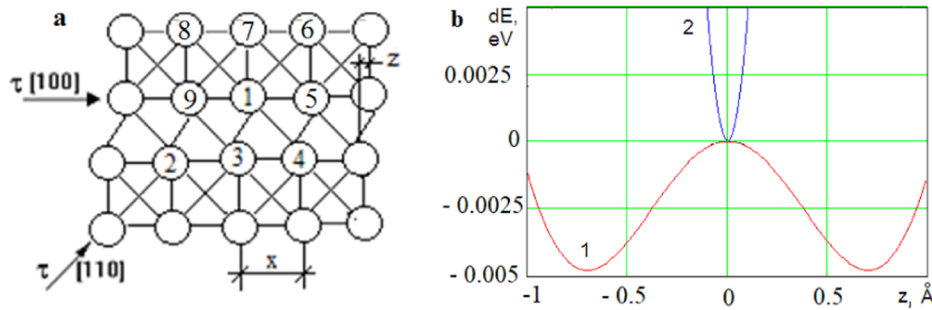
FIG. 3. Schematic of atomic plane shear in a two-dimensional crystal lattice (a). Change in atomic energy during shear in the [100] direction (curve 1) and [110] direction (curve 2) (b) at T = 0 K.[11] Adapted from L. Kozak, AASCIT J. Mater. **3**(5), 26–32 (2017). Copyright 2017 Association of Asian Scientific Journals for Material.

conduction band. This overlap causes the delocalization of electrons, resulting in high electrical conductivity.

The plasticity of metals is also attributed to the additional rapprochement of atoms. During compression, the potential energy of atoms increases by ΔU [Fig. 2(b)], causing them to occupy positions that do not correspond to their minimum potential energy. Consequently, with the simultaneous displacement of atoms in the [100] direction, their potential energy decreases [Fig. 3(b), curves 2]. This indicates the absence of resistance under the condition of the simultaneous displacement of all atoms exclusively in the [100] direction. However, in the [110] direction, shearing the atomic plane (curve 2) requires energy, indicating that the lattice is stable along this direction.

This phenomenon explains the low shear stresses and the selective shearing of atomic planes in real metals along crystallographic directions with the highest atomic density. Previous studies[9–11] have demonstrated that a compressed lattice is unstable, allowing atomic planes to shear under any external force.

It should also be noted that a dislocation is a region of a crystal where atoms are significantly displaced from their equilibrium positions.[7] Therefore, a dislocation represents a locally unstable region of the crystal, where atoms find themselves in positions that do not correspond to their minimum potential energy.

V. MODEL OF A PLASTIC CRYSTAL

Figure 4(a) presents a model of a plastic crystal with a two-phase structure.[6,21–23] The unstable crystal lattice is maintained in a state of unstable equilibrium by a surface layer (black atoms), whose structure and properties differ from those of the inner layer. Consequently, crystals with limited dimensions are stable under shear deformations, as the near-surface layers prevent the internal atomic planes from shearing. The strength of such crystals depends on the phase ratio.[21]

Consider the process of plastic deformation using the proposed model of a plastic crystal. When tensile stress is applied [Fig. 4(a)], the model suggests that these stresses are primarily absorbed by the surface atoms, while the internal atoms do not resist external loads. Upon reaching a critical stress level, the interatomic bonds of the surface atoms break. At the rupture point, the atomic planes [Fig. 4(b)] shear by one or more atomic distances through the slip mechanism. The ability of atoms to shear along the atomic plane over multiple interatomic distances is due to their

inertial motion, sustained by their potential energy until it is dissipated.

As a result of this shear, the internal atoms shear to positions of minimum potential energy [Fig. 3(b)]. Further displacement from these positions requires significant force. Consequently, the slip mechanism "transfers" to other atomic planes where no prior shear has occurred.

A further increase in stress will cause additional ruptures, leading to repeated displacements of atomic planes. Thus, the process of plastic deformation occurs through aperiodic shears of atomic planes.

This phenomenon is supported by experimental observations of unstable plastic deformation in metals and their alloys, which manifests as short-term stress jumps during tests on highly sensitive tensile machines. This effect is known as the Portevin–Le Chatelier (PLC) effect.[24,25]
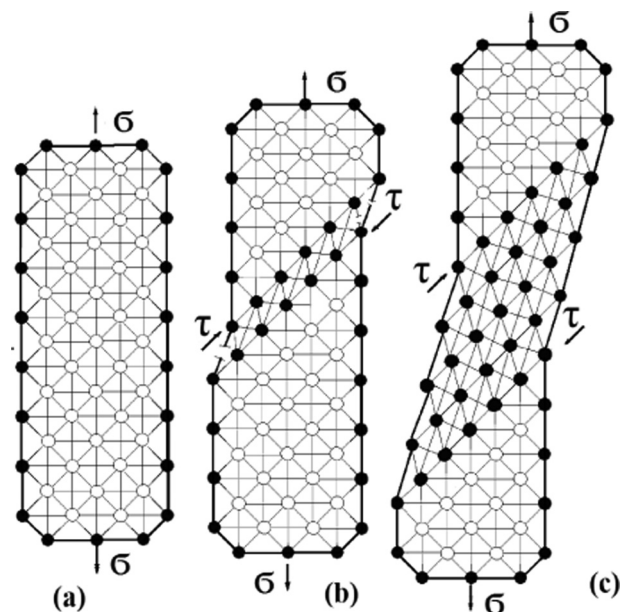

FIG. 4. Displacement of atomic planes in a single crystal (a) by the slip mechanism (b) and by twinning (c).
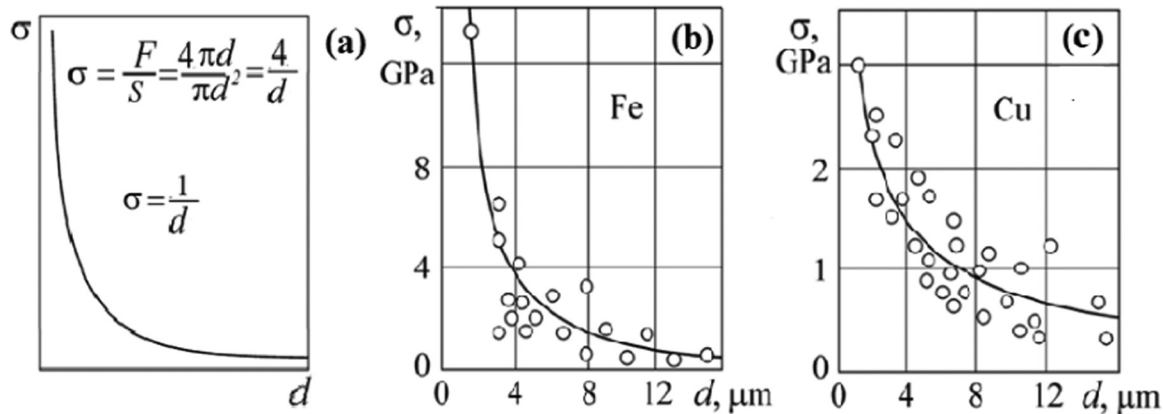
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FIG. 5. (a) Predicted curve of crystal strength as a function of crystal size. (b) Strength of iron "whiskers" as a function of diameter and (c) strength of copper "whiskers" as a function of diameter.[27] Adapted with permission from S. S. Brenner, J. Appl. Phys. **27**, 12 (1956). Copyright 1956 AIP Publishing LLC.

Another possible scenario involves the simultaneous shear of several atomic planes after the rupture of the surface layer [Fig. 4(c)] to a smaller interatomic distance, following the twinning mechanism. In this case, atomic plane displacement can occur without rupturing the surface layer. Instead, the interatomic distance within the surface layer will increase.

As a result of plastic deformation in shear regions, crystals become strengthened, and their structure undergoes significant modifications. Large metal single crystals fragment into nanocrystalline structures due to the shearing of atomic planes under the influence of minor external forces. This fragmentation enhances the crystal's strength. Thus, the transformation of a single crystal into a polycrystal occurs, where resistance to atomic plane shear depends on the size of subgrains and grains.[4,23]

It should be noted that the explanation of plastic deformation processes according to the proposed model differs from that provided by the dislocation model:

- The shear of atomic planes occurs [Fig. 4(a)] in the absence of any defects, as the crystal lattice itself is inherently unstable.
- Strengthening mechanisms during plastic deformation are explained by the movement of atoms to positions with lower potential energy [Fig. 3(b)].
- Atomic shear takes place simultaneously along the entire plane [Fig. 4(b)], leading to a disturbance in the crystal lattice structure.
- Shear occurs under low stresses, even in the absence of defects, including dislocations.

However, there are similarities between both models in explaining plastic deformation processes:

- The fundamental cause of plasticity is the instability of the crystal lattice. In the classical model, this instability is local, whereas in the proposed model, it is global.
- Plastic deformation results from the transformation of an unstable structure into a stable one, achieved through atomic

movement to positions of lower potential energy, as described in physical mesomechanics.[26]
- Plastic deformation occurs via slip and twinning mechanisms.
- The shear of atomic planes takes place under low stresses.

VI. EXPERIMENTAL CONFIRMATION

A. Depending on crystal strength of their size

According to the proposed model of a plastic crystal, its strength is determined by the strength of the surface layer and, thus, depends on the crystal size. At small diameters, strength is expected to be maximized and to decrease with increasing diameter, following the predicted curve [Fig. 5(a)].

Experimental results supporting this prediction are presented in Figs. 5(b) and 5(c).[27] Thin filamentary crystals, known as "whiskers," possess extraordinary strength. However, as the cross-sectional size increases, their strength decreases due to the diminished influence of the surface. At sizes greater than $50\,\mu$m, their strength approaches that of conventional technical metals.[27–31] In polycrystalline metals, strength also decreases with increasing grain size, following the Hall–Petch relationship.[32]

It should be noted that, according to dislocation theory, the high strength of whiskers is attributed to their ideal structure and is considered experimental confirmation of the classical concept. However, such assertions are inaccurate, as they fail to account for the surface of the whiskers, which acts as a two-dimensional defect.[33–35]

B. Single crystals with near-zero shear resistance

As the size of crystals increases further, their strength decreases to nearly zero. This conclusion is supported by studies of artificially grown, massive metallic single crystals characterized by high purity and a nearly perfect structure. These crystals exhibit exceptionally low shear resistance, approaching zero, providing

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direct evidence of the instability of their crystal lattice.[36–41] In p. 339 of Ref. 4, it is stated:

> "At the same time, single–crystalline metals are characterized by extremely low hardness in relation to planes and directions that are especially densely populated with atoms. This hardness (the yield point) of a single crystal that has not yet been subjected to any deformation after its manufacture does not exceed, particularly for vulnerable planes and directions, several tens of grams, or even just a few grams, per square millimeter. The question of the limit value of this softness cannot be considered definitively resolved. However, if we extrapolate the facts known today, it suggests that in an ideal crystal, which has not previously been subjected to any deformation, the initial hardness, at least for some planes and directions of plastic deformation, could be equal to zero."

It is important to note that the instability of massive metallic single crystals explains their absence in nature and the significant challenges associated with their growth under laboratory conditions. Information on these crystals remains relatively scarce, likely due to their inconsistency with the classical understanding of plasticity.

C. Higher strength of defective microcrystals compared to defect-free ones

As mentioned earlier, the strength of a defect-free crystal is determined by its surface layer, while the internal regions do not carry a significant load. However, during deformation, the internal layers of the crystal undergo strengthening as atoms shift to positions with lower potential energy. Therefore, if thick whiskers are carefully deformed, their strength should increase significantly.

These assumptions have been experimentally confirmed. In Ref. 28, the results of tensile deformation of three copper single crystals are presented, two of which have dimensions comparable to whiskers. One of the copper single crystals was deformed under very low stresses (1–5 MPa), yet the thick whisker exhibited significant strengthening (approximately 1200 MPa), which exceeded the elastic limit of the thin whisker (around 800 MPa).

This phenomenon is not an isolated case. Several additional experimental findings on the high strength of filamentous crystals and similar structures with a large number of defects are described in Ref. 30. These findings challenge the classical view that the high strength of filamentous crystals—whiskers—is solely a consequence of their ideal structure.

D. Confirmation of the simultaneous displacement of atoms

It can be assumed that the Portevin–Le Chatelier (PLC) effect serves as additional experimental confirmation of the proposed plasticity model. This effect is observed during tensile testing of metal samples using highly sensitive machines and manifests as discontinuous plastic deformation via slip and twinning. The PLC effect is characteristic of both pure metals and substitutional or interstitial alloys (e.g., mild steels, aluminum, and copper alloys).
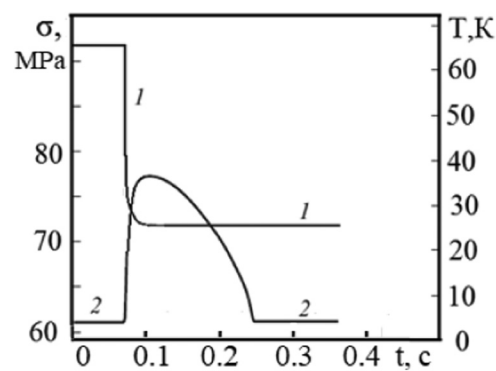

FIG. 6. Curves of stress drop (1) during a single jump and temperature rise (2) during the deformation of tantalum.[43] Adapted from Kuramoto et al., J. Phys. Soc. Jpn. **34**(11), 1217–1222 (1973). Copyright 1973 Physical Society of Japan.

Initially, these processes were observed in polycrystals,[24,25] but later, the effect was also reported in single crystals.[37]

For instance, in Ref. 25, the behavior and statistical characteristics of discontinuous deformation associated with the PLC effect were investigated in both single crystals and polycrystalline Al–Mg alloys. During the deformation of thin and bulk single-crystal samples, short-term stress jumps were observed at both normal[25] and low temperatures.[42,43]

According to the dislocation model, the shear of an atomic plane occurs through the successive displacement of individual atoms. In contrast, the new model suggests that atomic shear occurs simultaneously across the entire atomic plane.

Based on the proposed model, plastic deformation involves aperiodic displacements of atomic planes. Intermittent deformation manifests as jumps in stress and temperature.[42] The temperature jumps are attributed to the release of a significant amount of heat as atoms move to positions of lower potential energy. Figure 6[43] illustrates a unit jump in strain, evidenced by a drop in stress and a corresponding increase in sample temperature.

Notably, these effects are also accompanied by acoustic emission bursts, further corroborating the occurrence of simultaneous atomic shear.[44,45]

VII. INFLUENCE OF TEMPERATURE ON CRYSTAL LATTICE STABILITY

A. Theoretical investigation of shear resistance in atomic planes at different temperatures

Previous studies on a two-dimensional crystalline lattice[9,10] demonstrated that solids with a spherically symmetric interatomic interaction potential are unstable at 0 K [Fig. 3(b)]. This instability arises due to lattice compression, which causes the distance between nearest-neighbor atoms to become shorter than the equilibrium distance (Fig. 2). It is evident that temperature variations also influence atomic positions, thereby altering the state of the crystalline lattice.
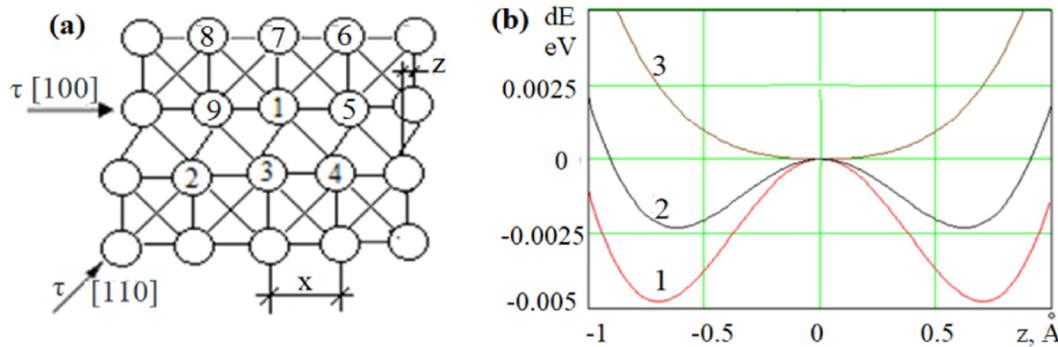
FIG. 7. (a) Scheme for calculating the energy expenditure. (b) Changes in potential energy during the shear of atom 1 by a distance z along the [100] direction within an atomic plane in crystals at different temperatures: T_1—curve 1; T_2—2; T_3—3; $T_3 > T_2 > T_1$.[11] Adapted from L. Kozak, AASCIT J. Mater. **3**(5), 26–32 (2017). Copyright 2017 Association of Asian Scientific Journals for Material.

Given this, the effect of lattice thermal energy on its stability was investigated. Under these conditions, atomic oscillations were considered a factor generating a repulsive force (internal pressure) between atoms, leading to an increase in the interatomic distance.

The objective of this study was to quantify the change in atomic energy during the shear of an atomic plane in the [100] direction at three different temperatures. The calculation scheme used is presented in Fig. 7(a).

Different temperatures were modeled by varying the interatomic distance within the crystalline lattice. Figure 7(b) illustrates the results of investigating the effect of temperature on the shear resistance of atomic planes in a two-dimensional crystalline lattice with a spherically symmetric interatomic interaction potential.

Graph 1 depicts the potential energy change of an atom during the shear of an atomic plane at a temperature of 0 K. At this temperature, the interatomic distance is minimal, $r_{01} = 2.34$ Å. Graphs 2 and 3 correspond to cases where the interatomic distance increased due to rising temperatures: $r_{02} = 2.45$ Å at temperature T_2 (curve 2) and $r_{03} = 2.6$ Å at temperature T_3 (curve 3).

Figure 7(b) (curve 1) also reveals that at temperature $T_1 = 0$ K ($r = 2.34$ Å), the crystal lattice is in a state of unstable equilibrium, as previously described (Fig. 3). This instability is attributed to the position of atom 1 at the "crest" of potential energy.

As the temperature increases, the interatomic distance grows to $r_{02} = 2.45$ Å. Consequently, the height of the "crest" on the potential energy curve decreases, as shown in Fig. 7(b), curve 2. At a higher temperature T_3, the interatomic distance increases further to $r_{03} = 2.6$ Å, causing the "ridge" to disappear (curve 3). This change in the potential energy profile indicates that energy is required to move the atom, demonstrating that at this elevated temperature T_3, the crystal lattice becomes stable.

Thus, at high temperatures close to the crystallization temperature (or the temperature of polymorphic transformation), the crystal lattice is stable. Crystals with such a lattice exhibit nonplastic behavior. Conversely, as the temperature decreases, the crystal lattice gradually becomes unstable due to compression, which increases the potential energy of its atoms. Crystals with an unstable lattice are plastic, and their plasticity increases as the temperature decreases.

The theoretical conclusions presented here are supported by the experimental data outlined below.

B. The region of low and middle temperatures

A number of researchers[46–52] have reported an increase in the plasticity of metals in the low and moderate temperature range. Confirmation of the theoretical results is presented in Fig. 8. The experimental stress–strain diagrams for aluminum[46] and copper[47] demonstrate an increase in plasticity with a decrease in temperature within the low and moderate temperature range.

Specifically, it was observed that as the temperature decreases from 350 to 4.2 K, the plasticity of metals increases, as evidenced by the greater relative elongation.

In a typical plastic metal lead, as a decrease in temperature from 265 °C to minus 271.5 °C, the relative elongation increases from $\delta = 20\%$ to $\delta = 46\%$. The same was observed during the study
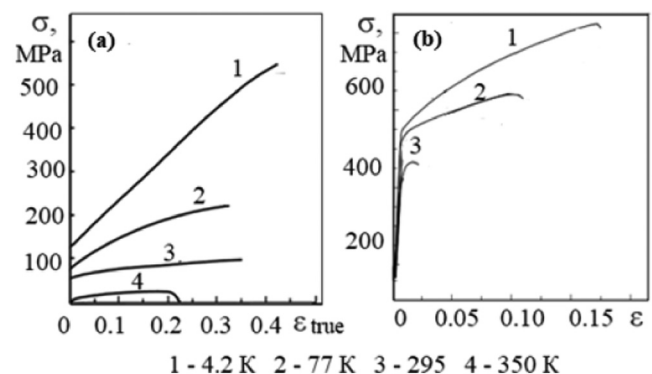

FIG. 8. Tensile diagrams of aluminum[46] (a) and copper[47] (b) deformed at different temperatures: 4.2, 77, 295, and 350 K. Adapted with permission from Estrin et al., Low Temp. Phys., **34**(8), 842–851 (2008). Copyright 2008 AIP Publishing LLC, and adapted with permission from Isaev et al., AIP Conf. Proc. 1783, 020121 (2016). Copyright 2016 AIP Publishing LLC.

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of single crystals of mercury with the identical Schmid factor (0.17). When the temperature decreased from −196 °C to −272 °C, the relative elongation of mercury increased from δ = 12% to δ = 89%.[48] Tin exhibited creep at temperatures lower than 1 K.[49]

The given experimental data indicate an increase in plasticity of pure metals with a decrease of temperature.

These experimental facts contradict Seeger's theory,[53] according to which plasticity should increase only in the event of rising temperature, as this is caused by an increase in the mobility of dislocations.

C. The region of high temperatures

It is widely recognized that the plasticity of metals and alloys generally increases with temperature. At elevated temperatures, plasticity is predominantly governed by amorphous-diffusion and intergranular-recrystallization mechanisms due to the high kinetic energy of atoms. However, experimental evidence indicates that plasticity can decrease at high temperatures.

This phenomenon, often referred to as "plasticity dips," has been observed in many metals, including those traditionally considered highly plastic.[48,54–56] Notable early researchers, including Le Chatelier (1901), Stribeck (1903), Yuza (1911), and others, identified one or more zones of brittleness ("plasticity dips") between room temperature and the melting point.[54]

For instance, experimental data show that the relative elongation of copper decreases from δ = 32%–62% at 20 °C to δ = 17%–29% at 500–600 °C, accompanied by a similar decline in narrowing, from ψ = 56%–60% to ψ = 17%–30%. Nickel exhibits analogous behavior, with elongation dropping from 13% to 15% at 20–300 °C to just 5% at 800–1100 °C.[54] Studies on iron and copper confirm this trend, showing that the relative narrowing of iron decreases from 76% to 4%–9%, and for copper, from 78% to 15%–38%, as temperatures rise to 700–900 °C. For purified and technical titanium, with increasing temperature from 200 to 500 °C, the relative

FIG. 9. Mechanical properties of as-received, HT60, HT160, and HT260 specimens tensile tested at 25, 500, and 800 °C.[52] Reproduced from Katiksiz et al., Metallophys. Adv. Technol. **43**(5), 673–688 (2021), licensed under a Creative Commons Attribution-NoDerivatives 4.0 International License.

elongation decreases from δ = 58% to 8% and from δ = 34% to 3%, respectively (Fig. 9).[48]

An alternative concept explains the low plasticity (plasticity drops) observed in the high-temperature range by the stable state of the crystal lattice, which causes its non-plasticity. Consequently, in this range, the intragranular material does not contribute to plastic deformation, while the amorphous intergranular regions exhibit low plasticity.

Below 500 °C, the crystal lattice transitions from a stable to an unstable state, thereby enabling plastic deformation. This transition alters the deformation mechanism from intergranular to intragranular. With a further decrease in temperature, the increasing destabilization of the crystal lattice results in enhanced plasticity of metals.

The increase in plasticity in the high-temperature region is attributed to a transition in the plastic deformation process from intragranular to intergranular, which is governed by amorphous-diffusion and intergranular-recrystallization mechanisms.

Thus, the proposed plasticity model aligns with experimental data on the effect of temperature on plastic deformation, whereas the dislocation model contains contradictions in its explanations of these findings.

VIII. CONCLUSIONS

- The geometry of the interatomic interaction potential is determined by the spatial distribution of valence electron density. Atoms with a spherically symmetric long-range interatomic interaction potential typically form an unstable crystal lattice, as observed in most metals. In contrast, atoms with an anisotropic potential characterized by directional bonds form a stable lattice, as in covalent and ionic crystals.
- The instability of the crystal lattice arises from a reduced interatomic distance compared to the equilibrium distance. This self-compression of the lattice is caused by a spherically symmetric long-range interatomic interaction potential.
- Solids with an unstable crystal lattice exhibit plasticity and are characterized by low resistance to shear under small deformations in specific crystallographic directions. In contrast, solids with a stable lattice are strong and non-plastic.
- The fundamental mechanism of plastic deformation involves the simultaneous displacement of all atoms in a plane to positions with lower potential energy, primarily via slip and twinning.
- Atomic plane displacements occur under low stress along crystallographic directions with the highest atomic density.
- The presence of defects in real metals—such as surface layers, grain and subgrain boundaries, dislocations, and vacancies—significantly increases shear resistance.
- Overall, the electronic structure of solids is the primary determinant of their plastic properties, while structural factors and environmental conditions play a secondary role.
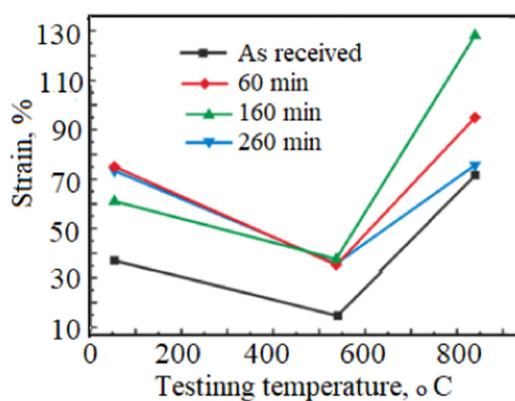
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AUTHOR DECLARATIONS

Conflict of Interest

The author has no conflicts to disclose.

Author Contributions

L. Kozak: Conceptualization (lead); Data curation (lead); Formal analysis (equal); Funding acquisition (lead); Investigation (lead); Methodology (lead); Project administration (lead); Resources (lead); Supervision (lead); Validation (lead); Visualization (lead); Writing – original draft (lead); Writing – review & editing (lead).

DATA AVAILABILITY

The data that support the findings of this study are available from the author upon reasonable request.

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