An Alternative Concept of Solids Plasticity

An Alternative Concept of Solids Plasticity

By

Liubomyr Kozak

Cambridge
Scholars
Publishing

An Alternative Concept of Solids Plasticity

By Liubomyr Kozak

This book first published 2025

Cambridge Scholars Publishing

Lady Stephenson Library, Newcastle upon Tyne, NE6 2PA, UK

British Library Cataloguing in Publication Data
A catalogue record for this book is available from the British Library

ISBN: 978-1-0364-5445-6
ISBN (Ebook): 978-1-0364-5446-3

With deep gratitude, I dedicate this work to my wife, **Nadiia Kozak**, for her unwavering support, inspiration, and invaluable technical assistance in the creation of this monograph. Her faith in me and her dedication have been an integral part of this journey.

> A trained specialist should remain free and independent in his thinking, and should avoid being limited by the temporal framework of publicly admitted knowledge in any science. It has to be remembered that the established science has already been forced many times to change or give up some of its most fundamental concepts.
>
> —Thomas S. Kuhn

The concept presented in this monograph belongs to the realm of revolutionary science and represents a departure from the traditional doctrine of plasticity. Unlike conventional approaches, which explain plasticity solely in terms of dislocations within a stable crystal lattice, the proposed framework emphasizes the fundamental role of the electronic structure and the intrinsic instability of certain lattices. In this paradigm, dislocations are not regarded as the root cause of plasticity but rather as local manifestations of lattice instability. Thus, the approach not only refines the classical view but also reconsiders its very foundations, offering an alternative explanation of the nature of solid plasticity and opening new avenues for further research.

CONTENTS

LIST OF FIGURES AND TABLES

Figures

Table

PREFACE

The phenomenon of plastic deformation is so widespread and commonly encountered in practice that it may seem extraordinarily simple and almost trivial. Virtually all metallic materials used in engineering and manufacturing experience plastic deformation at some stage, whether during processing, forming, or in their service life. The ability of metals to undergo plastic deformation under mechanical loads is fundamental to numerous industrial applications, from metal shaping and machining to the design of structural components capable of withstanding extreme conditions.

However, despite its apparent simplicity, metal plasticity remains one of the most complex and challenging phenomena to understand fully. This complexity arises from the intricate atomic and electronic interactions that govern plastic deformation, which vary significantly depending on external conditions such as temperature, pressure, and strain rate. As a result, even after decades of extensive research, many fundamental aspects of plasticity remain unresolved, continuing to be a subject of scientific investigation and debate.

Many studies have investigated plasticity, resulting in numerous models and theories. These include theories of dislocations, physical mesomechanics, plastic shear theories, models of jump–like propagation of plastic shear, and interactions of processes across various structural levels. Each of these approaches has contributed to our understanding of plasticity, yet none provides a fully comprehensive explanation. Despite numerous models and theories, we still lack a complete understanding of plasticity. Developing a unified physical theory remains especially challenging. This gap indicates the need for new hypotheses and theories that better explain the processes and phenomena associated with plastic deformation in solids.

This monograph introduces an alternative concept of plasticity, based on the idea of crystal lattice instability. According to this concept, depending on the electronic structure and external factors such as temperature and pressure, the ideal lattice of solids can be stable or unstable. solids with an unstable crystal lattice are not strong and are plastic, while solids with a stable crystal lattice is strong and non–plastic. The instability of a crystal lattice arises from self–compression due to specific interatomic interactions. In an unstable lattice, atoms occupy positions that do not correspond to their minimum potential energy. Plastic deformation, in this view, is the process by which an unstable crystal lattice transforms into a stable structure, with atoms moving to positions of lower potential energy.

This alternative concept contradicts the modern concept in the physics of strength and plasticity, which regards the ideal crystal lattice of solids as resistant to shear deformation and thus non–plastic. In the modern view, high stresses are required to shear the atomic planes, and plastic deformation is possible only in the presence of specific defects, such as dislocations. Dislocations are defects in the crystal lattice caused by atomic deviations from equilibrium positions, enabling the displacement of atomic planes at low stresses. Essentially, dislocations represent local instability within a stable crystal lattice.

In contrast, the alternative concept proposed here views the ideal crystal lattice of plastic materials as inherently unstable in its initial state, thereby eliminating the need to introduce local instabilities (such as dislocations) for plastic deformation to occur. Consequently, the process of plastic deformation is significantly simplified: it is simply the transformation of an unstable lattice into a stable structure, with atoms moving to positions of lower potential energy.

The implications of this alternative approach extend beyond materials science and the physics of strength and plasticity. A deeper understanding of lattice instability could lead to new strategies for designing materials with tailored mechanical properties, enhancing their strength, ductility, and resistance to failure. Additionally, this concept may provide insights into deformation mechanisms in nanostructured materials and amorphous solids.

Overall, plastic deformation–whether explained by the classical or alternative concept–is a consequence of instability. However, the classical approach considers this instability to be local, while the alternative approach views it as global. By re–examining the fundamental nature of plasticity through the lens of crystal lattice stability, this work aims to offer fresh perspectives that could contribute to the development of a more unified and comprehensive theory of plastic deformation.

ACKNOWLEDGMENTS

I would like to express my heartfelt gratitude to V.Ya. Bilousov, O.V. Pylypchenko, L.S. Livshits, O.T. Cirulnyk, O.M. Romaniv, M.M. Student, Y.V. Zima, O.I. Balytskyi, P.I. Melnyk, M.O. Galushchak, Y.A. Kryl, D.M. Freik, Y.P. Saliy, O.M. Ivasyshin, E.I. Kryzhanivskyi, Yu.Ya. Meshkov, S.A. Kotrechko, S.P. Oshkaderov, O.E. Andreykiv, Y.L. Ivanytskyi, M.G. Staschuk, and L.Ya. Ropyak. I especially remember those colleagues who have passed away.

These scientists provided invaluable advice, support, and constructive criticism throughout the development of this monograph.

I am also grateful to everyone who attended the seminars where I presented my findings, including those at Vasyl Stefanyk Karpattia University, the H.V. Kurdyumov Institute for Metal Physics, and the H.V. Karpenko Physico–Mechanical Institute. Their insights and discussions have greatly contributed to the development of this work.

Special thanks to my wife, Nadiia Kozak, for her unwavering moral support.

Without their encouragement, the creation of this new concept would not have been possible, as the research presented in this monograph ventures beyond the bounds of traditional science into the realm of revolutionary science, associated with paradigm shifts. Such groundbreaking work often receives cautious and critical reactions, requiring extended contemplation and thorough study.

Work on the alternative concept of plasticity began a long time ago. From my initial “immature” ideas to the formation of the concept and the writing of this monograph, nearly half a century has passed. This journey involved extensive searches for empirical and theoretical evidence, thorough analyses, and countless discussions with colleagues, both informally and in formal seminars.

The driving forces behind these efforts were curiosity and the desire to validate my ideas. The joy and euphoria of confidence in being correct were often replaced by disappointment and discouragement due to harsh criticism. Such criticism, while natural for studies of this kind, was not always fair. However, the support and assistance of colleagues continually inspired me to further my search, for which I am deeply grateful to them.

With great respect and gratitude,

Liubomyr Kozak

CHAPTER 1

INTRODUCTION

The modern physics of strength and plasticity is based on the concept of the stability of the crystal lattice of solids. Displacement of the atomic planes in a crystal lattice of an ideal structure requires extremely high shear stresses. This means that the ideal crystal lattice of solids is resistant to shear deformation. The strength of such a lattice is extremely high. The basis for such views is the high values of the modulus of elasticity of solids. However, the experimental values of the shear resistance of the atomic planes are two to three orders of magnitude lower than the calculated values obtained from the classical shear model of Ya.I. Frenkel.

These stresses are particularly low for massive metal single crystals of high purity and perfect structure. Such crystals plastically deform at very low stresses, close to zero.

To eliminate the inconsistency between the theoretical calculations and experimental data, a separate model of plastic deformation was created. According to this model, the perfect crystal lattice has specific defects, i.e., dislocations. Their presence, as well as their nucleation in the process of plastic deformation, contributes to the shear of atomic planes under the action of relatively small external stresses. It is believed that plastic deformation is impossible without dislocations.

The dislocation model was proposed by Taylor, Orowan and Polanyi in the 1930s and is widely recognized today. At one time, the dislocation model was harshly criticized, but the critical attitude toward it did not prevent its spread and recognition. However, for more than a century, a significant amount of experimental and theoretical research has accumulated that is difficult to explain solely on the basis of dislocation theory. Some of these explanations are very complex and even contradictory. According to the current view, dislocation theory can be used only for a limited number of simple explanations of certain partial models of plastic deformation. For a complete description of macroplastic deformation of solids, it is necessary to introduce spatial structural elements of deformation that can not only move but also rotate during motion. This led to the creation of a number of plasticity models of solids, the authors of which are G.V. Samsonov, V. I. Arkharov, V. V. Panasuk, Yu.Ja. Meshkov, V.I. Zasimchuk, V.E. Panin, V.A. Likhachev, V.V. Rybin, R. Hill, W. Prager, V.V. Neverov A.I. Antonenko and others.

However, all new hypotheses and theories are also based on the concept of the high stability of an ideal crystal lattice. This applies to brittle and nonplastic solids as well as highly plastic solids, regardless of the type of chemical bond.

The monograph proposes a new model of the plasticity of solids on the basis of an unstable crystal lattice. According to an alternative concept, an ideal crystal lattice can be in a stable or unstable state. The state of the crystal lattice depends on the shape of the interatomic interaction potential and external parameters, such as temperature and pressure.

The shape of the potential, which is spherically symmetric or asymmetric, is determined by the nature of the distribution of the electron density in space. In the case of a spherical potential, solids with an unstable crystal lattice are formed. But in the case of an asymmetric potential, solids with a stable lattice are formed. The existence of solids (crystals) with an unstable crystal lattice is due to the presence of a thin surface layer and internal defects. The structure and properties of the surface layer are radically different from those of the inner regions of an ideal crystal lattice.

Solids with an unstable crystal lattice are in a state of unstable equilibrium. Their internal atoms are in positions that do not coincide with the positions of minimum potential energy. The process of plastic deformation of such solids is considered as the process of moving atoms to positions with lower potential energy under the influence of external forces. Solids with an unstable crystal lattice are highly plastic (metals) in contrast, to nonplastic solids with a stable lattice (for example, diamond crystals).

At first glance, it may seem that the concept based on an unstable crystal lattice, is suspicious and also did not correspond to reality. However, the classic concept of a stable crystal lattice at one time also did not correspond to reality. Overall, the shear stress of the atomic planes in such a lattice is two to three orders of magnitude greater than that in real metals and their alloys. Therefore, a dislocation model was created to resolve these discrepancies.

Notably, according to the alternative concept of plasticity, the existence of dislocations in the crystal lattice and their movement during deformation is not denied. However, according to an alternative concept, the processes of nucleation and movement of dislocations occur as a result of the shear of atomic planes, not vice versa. Dislocations are not the cause of the easy shear of atomic planes but the instability of the crystal lattice.

In general, according to an alternative concept, plasticity is a property of a defect–free crystal lattice. The fewer defects there are, the greater the plasticity of the crystals and the lower their strength. This point of view was also held by other researchers. At one time, Ya.I. Frenkel, A.V. Stepanov, M.V. Klassen–Neklyudova, T.A. Kontorova believed that the ability to undergo plastic deformation is one of the main properties of a defect–free crystal lattice of metals, whereas according to dislocation theory, a crystal that does not contain dislocations does not show plastic properties at all.

Since, according to an alternative concept, the defect–free crystal lattice of metals is unstable, the shear of atomic planes in it occurs under any small external forces. The presence of surface, grain and subgrain boundaries and internal defects in real crystals creates resistance, to the shear of atomic planes, so the fewer defects there are, the more plastic real crystals are.

It is well known that dislocations in an ideal crystal lattice are atoms displaced from positions with minimum potential energy (from their equilibrium positions). That is, dislocations are local unstable formations in a stable crystal lattice. This means that the dislocation model is based on instability, as in the proposed model. The process of plastic deformation due to the movement of dislocations is also a process in which atoms move from an unstable position to a stable one under the influence of external forces.

In addition, the process of plastic deformation, both according to the dislocation model and the proposed model, occurs via the same mechanisms: slip and twinning. For both models, the process of plastic deformation is the displacement of atoms to positions with lower potential energy.

The alternative concept of solids plasticity is more fundamental than dislocation theory and other modern hypotheses and theories of plasticity. According to this concept, plasticity is caused by the instability of the crystal lattice, which occurs in solids with a spherically symmetric potential of interatomic interaction. Moreover, the shape of the interatomic interaction potential is determined by the distribution of the density of valence electrons in space. In general, the plasticity of solids depends on their electronic structure.

CHAPTER 2

FEATURES OF PLASTIC DEFORMATION OF SOLIDS

2.1. Types and mechanisms of plastic deformation

The phenomenon of plastic deformation is an irreversible change in the shape of solids under the influence of external forces. Unlike elastic deformation, plastic deformation is residual and persists after the removal of the load. It is associated with the movement of atoms inside over a certain distance from one equilibrium position to another, causing residual changes in shape, structure, and properties without macroscopic violations of the material's integrity. A distinction is made between the plastic deformation of amorphous bodies and crystalline bodies, mainly metals [1, 2].

The processes of plastic deformation during cold and hot metalworking differ. Accordingly, the following types of plastic deformation are distinguished:

- Athermal (diffusion–free) plasticity.
- Thermal (diffusion) plasticity.

The term “athermal plasticity” is used because it can occur at temperatures close to absolute zero. It is more appropriate to use the term “crystalline plasticity” since it occurs in crystalline materials, such as metals and some minerals. Such plastic deformation is caused by the shear mechanism, i.e., slip and twinning.

Crystalline plastic deformation is the simplest type of plastic deformation of crystals and occurs via the shear of atomic planes along the crystallographic directions.

The monograph deals mainly with crystalline (athermal) plastic deformation. Its features include:

–shear of a plane occurs only in strictly defined crystallographic directions;
–the process of plastic deformation is accompanied by the strengthening of metals;
–plasticity of metals can occur at low temperatures (down to 0 K).

At high metal processing temperatures, mechanisms of thermal plasticity come into play [2]. The mechanisms of thermal plasticity include the following:

–Amorphous–diffusive.
–Intergranular–recrystallization.
–Interphase solution–precipitation.

The intergranular recrystallization mechanism is based on the formation of new recrystallized grains and the healing of defects during deformation at high temperatures. This mechanism is characteristic of "pure" metals and single–phase alloys, where the absence of impurities promotes the mobility of grain boundaries and facilitates recrystallization [3].

The interphase solution–precipitation mechanism occurs in multiphase alloys. During deformation, damage at the boundaries of phases with high mutual solubility is healed, allowing stress accommodation through the interaction of different phases [4]. It is important to note that mechanisms of thermal plasticity are significant during hot pressure processing, where high temperatures enable processes such as recrystallization and diffusion. However, their influence is negligible during cold pressure processing, where plastic deformation primarily occurs via the shear mechanism, including slipping and twinning. These mechanisms are essential for understanding the plastic deformation of metals and crystals.

2.2 Early concepts of plastic deformation

Although plastic deformation is a common phenomenon, it remains one of the most complex and intriguing processes in materials science. Understanding its nature required significant advances in the fundamental sciences. Only after the development and experimental validation of atomic and nuclear theories, the formulation of quantum mechanics and electronic theory of metals, and studies of other crystal properties, such as magnetism and electrical conductivity, did the understanding of plastic deformation begin to take shape.

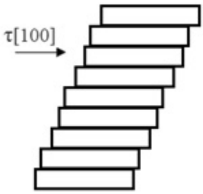

Fig. 2.1. Boas–Schmid model [1]

Early researchers studying the plastic deformation of metals proposed that it occurred through the shear of one atomic plane relative to another. This concept was illustrated by the Boas–Schmid model (Fig. 2.1), where the movement of atomic planes was compared to the slip of a stack of coins.

In this model, the shear of atoms was thought to happen simultaneously across the entire atomic plane. However, this simplistic representation posed a significant problem. The theoretical values of the critical stress required for such shear were calculated to be 3–4 orders of magnitude higher than the experimental values measured for technical metals.

By the 1930s, this discrepancy highlighted a fundamental challenge in materials science: explaining the mechanisms of plasticity at the microscopic level. The simplified approach to calculating shear stress proved inadequate, underscoring the need for more sophisticated hypothesis to describe the complex nature of atomic–scale deformation.

Ya.I. Frenkel calculated the shear stresses required for the displacement of atomic planes in a crystal [4]. He analyzed a simplified model involving two rows of atoms slip relative to one another under shear stress. For a material with a shear modulus G, the shear strength is approximately determined by the following formula:

$$\tau_m = \frac{G}{2\pi} \approx \frac{1}{6} G$$

The shear modulus of metals is typically in the range of 20,000–150,000 MPa, indicating a predicted shear stress of 3,000–25,000 MPa. However, the actual measured shear stresses range from 0.5–10 MPa.

For example, for copper, the shear modulus value is $G \approx 46000$ MPa, and the theoretical shear stress values are $\tau_m \approx G/6 \approx 7600$ MPa. The experimentally determined (at 20 °C) critical shear stress $\tau_m \approx 1$ MPa, i.e., 7600 times greater. The same is true for other metals. For single–crystal metals, the critical shear stress is even lower, approximately $\tau_m \approx 0.01–0.1$ MPa.

According to calculations, deforming an ideal crystal requires exerting an exerting a large effort, as it involves simultaneously shearing all the atoms in the plane. However, the actual strength of materials is three to four orders of magnitude lower than the calculated values.

To resolve the significant discrepancy between the theoretical and actual strengths of materials, a dislocation model of plasticity was developed [4–7]. This model proposes that real crystals contain specific defects, known as dislocations, which significantly reduce the critical shear stress required for plastic deformation τ_m.

According to the scheme (Fig. 2.2), the atoms of the crystal lattice are located on the bottom of the potential relief. To displace them, it is necessary to “roll” each atom thru the “top” of the relief. It is evident that simultaneous shearing of all atoms would require significantly more energy than sequential, individual shearing of atoms. These observations formed the basis of the dislocation model.

According to the dislocation mechanism of plastic deformation, the energy of external stresses is transferred sequentially from one atom to another. The relay–like nature of energy transfer facilitates the shearing of atomic planes with much less energy consumption.

In plastic materials, dislocations serve as the 'carriers' of plastic deformation, and the energy required to move these dislocations is significantly lower than the energy needed to shear atomic planes in an ideal crystal lattice.

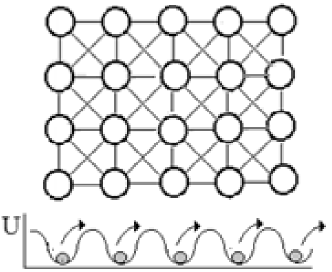

Fig. 2.2. Potential relief in the classic lattice

2.3 Dislocation model of a plastic crystal

Dislocations are formed during the crystallization of metals from groups of vacancies and can also be generated during plastic deformation and phase transformations. An important characteristic of dislocations is their density, which is defined as the total length of dislocations (in centimeters) per unit volume of the crystal (centimeters ^{3}).

A dislocation is a region in a crystal near an incomplete atomic plane, where atoms are significantly displaced from their equilibrium positions (Fig. 2.3a). The simplest type of dislocation is an edge dislocation, which is a linear defect. If a single crystal is cut along plane N to line AB and a stress τ is applied to its upper part, the upper part will move relative to the lower part, forming an additional atomic plane with an edge at AB (Fig. 2.3a).

Macroscopically, a dislocation represents the boundary KL that separates the portion of the crystal where shear has occurred from the portion where shear has not yet occurred (Fig. 2.3b).

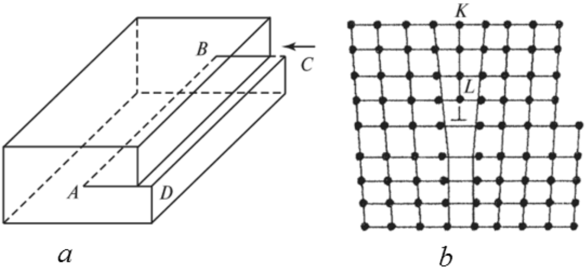

Fig. 2.3. Edge dislocation–***a*** and its schematic representation in the crystal lattice–***b*** [7]

The energy barrier for dislocation movement decreases as the distortion zone around the dislocation increases. Based on the mobility of dislocations, all materials can be divided into two groups:

1. Covalent crystals: In these materials, the energy barrier for dislocation movement is close to the energy of interatomic bonds and can only be overcome via thermal activation (thermal fluctuations). As a result, the mobility of dislocations becomes significant only at sufficiently high temperatures. At moderate temperatures, covalent crystals exhibit low plasticity and behave as nonplastic materials.

2. Metals and ionic crystals: In these materials, the energy barrier for dislocation movement is 10^3–10^4 times smaller than the binding energy and vanishes under stresses of 10^{-3}–10^{-4} G (where G is the shear modulus). Under such low stresses, dislocation movement does not require thermal activation, and their mobility is only weakly dependent on temperature. The low resistance to dislocation movement in ideal crystal lattices explains the high plasticity of metals.

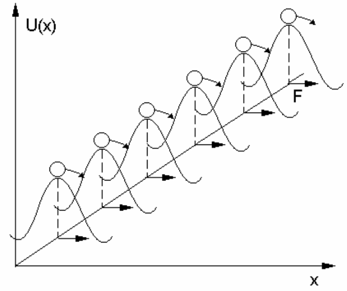

Fig. 2.4. Potential energy of atoms in the dislocation core [7]

In general, a dislocation represents a group of atoms located at the crest of a potential barrier (Fig. 2.4). This allows for plastic deformation of the crystal under the influence of relatively small external stresses [7].

The elementary act of plastic deformation can be explained by an edge dislocation–the shear of an atomic plane by one interatomic distance. However, to sustain further shear, the formation of new dislocations is necessary. To describe this process, complex mechanisms have been developed, including the generation of dislocations by the Frank–Read source and dislocation creep.

Additional models of dislocations include helical, twin, vertex, grain boundary, single, partial, prismatic, stretched dislocations [5, 6] and other.

The theory of dislocations serves as the foundation of modern physics of strength and plasticity [4–7]. The dislocation model, proposed by Taylor, Orowan, and Polanyi in the 1930s, is widely recognized today. However, over the past century, a significant body of experimental and theoretical research has accumulated, much of which is challenging to fully explain using dislocation theory alone. Some interpretations within the framework of this theory remain highly complex and, at times, even contradictory.

Although the dislocation model faced severe criticism at one time, this critical attitude did not hinder its widespread adoption and recognition. To date, no superior atomic model has been proposed that can better explain the phenomenon of low shear stresses in atomic planes of an ideal crystal lattice.

2.4 Limitations of the dislocation model of plasticity

In the last century, the discovery and study of dislocations shaped our understanding of deformation and plasticity. Yet the dislocation model and theory faced criticism, usually divided into two periods: the 1930s–1950s, during its emergence, and after the 1970s, during its refinement.

The early opponents of the dislocation model of plasticity included Ya.I. Frenkel [4], A.V. Stepanov [8], M.V. Klassen–Neklyudova, and T.A. Kontorova [9], among others. Later, researchers such as V.E. Panin [10], V.A. Lykhachev [11], V.I. Vladimirov [12], V.V. Rybin [13], V.I. Zasymchuk [14], as well as Hutchinson, Peirce, Becker, Kocks, Arsenlis, Parks, Ma, Roters, and others [15–17], joined them. While offering constructive criticism of the dislocation model, these researchers also proposed new models of plastic deformation.

In the early development of ideas about the strength of metals, most researchers concluded that the discrepancy between theoretical calculations and the real strength of metals was due to the presence of specific defects, i.e., dislocations.

Opponents of the dislocation model argue that the ability to undergo plastic deformation is a fundamental property of an ideal crystal lattice in metals [8, 9]. According to their view, an ideal crystal lattice of a metal should inherently possess high plasticity. In contrast, the dislocation model maintains that plastic deformation is possible only in a defective crystal lattice containing specific defects, whereas an ideal lattice does not exhibit plasticity.

However, experimental observations have convincingly demonstrated that the more perfect the structure of a crystal, the greater its capacity for plastic deformation [9]. For example, the slower a single crystal grows from a melt, the more perfect its structure becomes, and the lower its elastic limit. Annealing and relaxing crystals have also been shown to sharply decrease the elastic limit. Additionally, it is well established that the purer a single crystal is, the fewer impurities it contains, and the more plastic it is. Any distortions in crystals–such as transition zones, grain boundaries in polycrystals, or mosaic block boundaries in single crystals–consistently act as obstacles to plastic shear. Based on these observations, the aforementioned facts clearly contradict the foundational assumptions of the dislocation theory of plasticity [9].

In general, the opponents of the dislocation model did not deny the existence of dislocations in crystals. In fact, it was acknowledged that both edge dislocations and screw dislocations can form during the crystallization of real crystals. However, they rejected the idea that dislocations possess a unique property of mobility that distinguishes them from all other crystal lattice defects. According to these critics, dislocations are not directly involved in the occurrence of plastic shear but instead act as obstacles to plastic deformation [9].

According to their views [4, 8, 9], the main characteristic feature of crystals is the correct and the correct and regular arrangement of their atoms or ions, not the presence of defects of any particular type. Moreover, the ability to undergo plastic deformation is one of the specific inherent of crystalline bodies. They attempted to build a physical theory of crystal plasticity on the basis of the properties of a regular crystal lattice [4, 8, 9]. However, they failed to create an atomic model that would explain the ease of shearing of atomic planes under slight stresses, similar to how it is explained by the dislocation model. Therefore, the assumption that plasticity is a property of the crystal lattice was not accepted.

Until 1980, the traditional description of plastic deformation of crystalline solids was conducted within the framework of dislocation theory [3–7]. The most common point of view is that total plastic deformation results from the relatively independent motion of individual dislocations. Displacement of dislocations is believed to be additive. The basis of this is the Taylor scheme, which allows the action of five slip systems in the crystal to provide any change in its shape without breaking its integrity. However, later works [10–12] testify to the impossibility of the Taylor scheme in some cases. Thus, preserving the integrity of the material in the case of no coincidence of the directions of the applied stresses and crystallographic slip requires the activation of rotational modes of deformation. Since translational motion of dislocations cannot generate rotational effects, such modes are not accounted for in classical dislocation theory. At the same time, reversible modes of deformation are observed in many cases. These are, for example, rotations of individual blocks at large strains, as well as rotations of individual grains during plastic deformation at high temperatures and rotational motions in polycrystals under superplastic flow conditions. The explanation of these processes by dislocation slip at a high density of dislocations is problematic, so it is necessary to proceed to disclinations [12, 13].

It was shown in [14] that, under certain conditions, the dislocation mechanism of crystal plastic deformation transitions into the hydrodynamic flow of material through channels with a disordered (liquid–like) internal structure. This process is caused by instabilities that arise during the deformation of the dislocation structure and the self–organization of defects in the crystal lattice. These defects form so–called hydrodynamic flow channels, which are oriented along the directions of the maximum components of the applied stress tensor.

After rapid development between the 1930s and 1970s, interest in dislocation theory declined. Initially, it was believed that solving the mathematical challenges of describing dislocation ensembles would allow theoretical calculation of macroscopic properties of deformed solids. However, accumulated experimental data showed that the classical theory applies only to limited, simple cases, such as partial models of plastic deformation or material failure.

Attempts to establish a direct connection between the microscopic level physics of dislocations and the macro–level mechanics of materials have proven unsuccessful. In recent decades, it has become clear that such attempts are fundamentally unpromising. Despite numerous serious efforts, the consistent use of dislocation theory to develop a comprehensive theory of macroscopic mechanical properties has failed [10].

Dislocation theory has not yielded a comprehensive framework for describing macroscopic mechanical properties. However, the knowledge of atomic–scale mechanisms and processes remains insufficient for accurately describing and predicting the plastic deformation of macroscopic bodies.

2.5 New models of solids plasticity

Currently, additional approaches have been developed to describe plastic deformation [10–17]. These main models consider plastic deformation as a loss of stability due to external forces. According to these authors, plasticity arises from the instability of the crystal lattice under an applied external force. Mechanical instability refers to a partial or complete loss of the material's ability to withstand applied loads, with ordinary plastic deformation being one form of this mechanical instability. In general, a connection between plasticity and instability has been noted in several studies [18–25].

V. Panin [10] and colleagues created physical mesomechanics. According to its provisions, plastic deformation and destruction of solids are connected with the loss of their stability under shear deformation at different scale levels, where strongly unbalanced states of the crystal lattice arise. These processes are of a relaxation nature.

In general, according to modern models, the process of plastic deformation occurs in two stages. Under the action of an external force, regions of unstable structure (various defects, including dislocations) form within an ideal lattice. The second stage is the transformation of an unstable structure into a stable one. These processes occur simultaneously and continuously during plastic deformation. Under the action of an external force, atoms first move to a state of higher potential energy, and then to one of lower potential energy.

Thus, all new models of plasticity are based on the classical concept of the stability of an ideal crystal lattice.

Despite numerous hypotheses and theories, the dislocation model remains the only one that explains the significant discrepancy between theoretical and actual shear stresses in the atomic planes of metals. However, this model is based on concepts and knowledge developed over a century ago. Since then, substantial advancements have been made: theories of the atom and atomic nucleus have been established, the foundational principles of quantum mechanics and the electronic theory of metals have been formulated, and various properties of crystals, such as magnetism and electrical conductivity, have been studied. Additionally, the influence of environmental factors–such as extreme temperatures and high hydrostatic pressure–on plastic deformation processes has also been investigated. Therefore, a contemporary explanation of the phenomenon of plastic deformation in solids is incomplete without integrating these new insights.

Existing models of solids often fail to account for changes in their electronic structure. This approach is overly simplistic, as real atoms have geometric dimensions determined by their electron shells. When atoms are displaced by external forces, complex interactions arise that can significantly influence the electronic structure of solids. These interactions lead to both quantitative and qualitative changes in interatomic forces, ultimately affecting the mechanical properties of solids. Therefore, such factors must be considered when studying complex phenomena like plasticity.

CHAPTER 3

PREREQUISITES FOR DEVELOPING AN ALTERNATIVE CONCEPT OF PLASTICITY

3.1 Influence of electronic structure on the mechanical properties of solids

In the physics of strength and plasticity, defects in the crystal lattice are believed to play a pivotal role in the formation of the mechanical properties of solids–namely, strength and plasticity. These properties are traditionally considered to depend on the structure of solids, without relating these characteristics to their electronic structure. However, the propensity of solids to deform plastically depends not only on the presence of specific defects, such as dislocations, but also on their electronic structure (the type of chemical bond). Metals exhibit the highest degree of plasticity. Conversely, most crystalline bodies with covalent and ionic bonds tend to have low plasticity. Notably, the type of chemical bond is the primary factor determining the plasticity of solids, whereas the structural factor is secondary. Indeed, dislocations are present in ionic and covalent crystals as well as metals, but high plasticity is characteristic only of metals. Additionally, metals are the most effective conductors of electric current.

According to an alternative concept, the property of plasticity is related primarily to the electronic structure of solids (type of chemical bond) and not only to their structural factor. This is an important difference between the alternative concept and the existing one.

In many models of solids, atoms are considered as material points with interaction forces acting between them, and they are displaced from their equilibrium positions when deformed. However, as noted above, these models often do not account for changes in the electronic structure, making this approach overly simplistic. In reality, atoms have geometric dimensions determined by their electron shells. When atoms are displaced, complex electronic interactions can occur, leading to changes in interatomic forces, which, in turn, influence the mechanical properties of solids.