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Elongation and shortening under elastic deformation at atomic level

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ABSTRACT: *The problem of changing and restoring sizes of a solid body under an elastic deformation is considered. A model of mutually penetrating atoms for description of atomic structure of a condensed matter is used for the analysis of the phenomenon at atomic level. Schemes of the model atoms, rules of their approaching during formation of atomic structures, appearance of Coulomb attractive forces between atoms are given. Shown is the scheme of appearance and action of interatomic forces that provide the change of size and shape of a solid body during elastic deformation, and their restoring after releasing the external stress.*

Keywords – *atomic cell, elastic deformation, interpenetrating atoms, elongation, contraction*

I Introduction

At small stress, solid bodies undergo an elastic deformation. This means that after releasing the external forces, the shape and sizes of the body return to previous ones.

At elastic strain, a body elongates in the axis of applied load. Its cross-section decreases in accordance with a Poisson coefficient. But why the contraction of the sample occurs? This question is not fully answered in the scientific literature. The problem is in the fact that it is not clear how forces contracting the sample appear and act. At the elastic uniaxial compression the body expands in perpendicular directions. How appear forces perpendicular to the compressing force, that are expanding the compressed body?

In the paper presented, these questions are considered at the atomic level. It is shown how electrostatic atomic interactions can appear in the condensed matter and ensure the contraction of the atomic cell during elastic elongation and its expansion during uniaxial compression.

II Interpenetrating atoms and their self-organization

2.1 Problems in forces shifting atoms during elastic deformations

The distance between atoms during elastic tensile stress increases in the direction of the load acting upon the object, Fig. 1. But how and from where appear the forces that decrease the distance between atoms in the transverse direction?

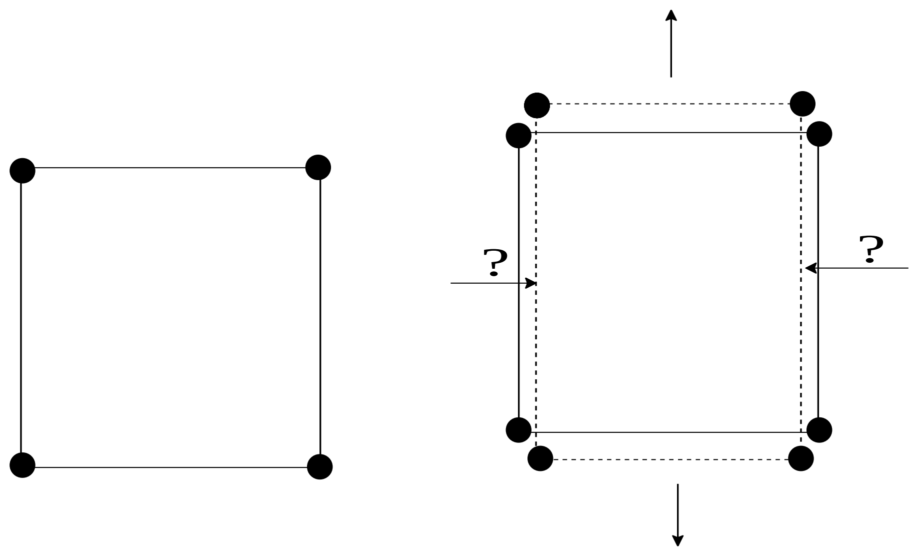

Fig. 1. The scheme of shifts of the atomic centers at elastic tensile stress (dashed lines).

And what happens when there is no already a tensile force? From where and how appear the forces that move atoms in the opposite direction and restore the initial distances between the atoms?

And even more puzzling problem: from where appear forces that, after vanishing the tensile forces, ensure the increase of the distance between atoms in the direction perpendicular to the elongation?

These questions are so evident and urgent that if the modern theory could only had obtained convincing answers they would have been obtained. They would have been widely known and entered handbooks and textbooks. But there are no answers.

The presented paper describes an attempt to answer these questions using a model of mutually penetrating atoms for the formation of atomic structures of condensed substances [1-4].

2.2 Quantum-classical model of atoms and their packing.

In the author's papers [1-2], a geometrical model of atoms and a rule of their packing have been suggested, which allow one to model the formation of atomic cells and crystal structures that are typical for substances with different types of interatomic bonds: the metallic (for bcc and hcp lattices), covalent (of the graphene and diamond type), ionic (of the NaCl type) bonds and other. Using this geometrical model and the rule and taking into account modern physical concepts, a combined quantum-classical model of atoms and a universal mechanism of joining of atoms into a condensed substance have been proposed [3, 4]. The classical properties of the combined quantum-classical model of atoms include mass, electric neutrality, certain sizes and shape, thermal vibrations, and, the main, well-defined space position of atoms relative to other atoms in condensed substances (in crystal and molecular structures). Quantum properties manifest themselves in the fact that a mutual penetration of atoms is possible, but the filling by electrons in accordance with the Pauli exclusion principle, that is obligatory for single (free) atoms, is also set for atoms in a condensed substance.

The atomic shell of outer electrons (in Fig. 2 it is bounded by a circle of dashed line) is not completely filled by electrons. So, the electrons from other atoms can penetrate it. But according to the Pauli rule, the electron spins in the shell and, correspondingly in the interpenetration region, should be different. Therefore, the mutual penetration can be only pairwise (the atoms 1 and 2 in Fig. 2).

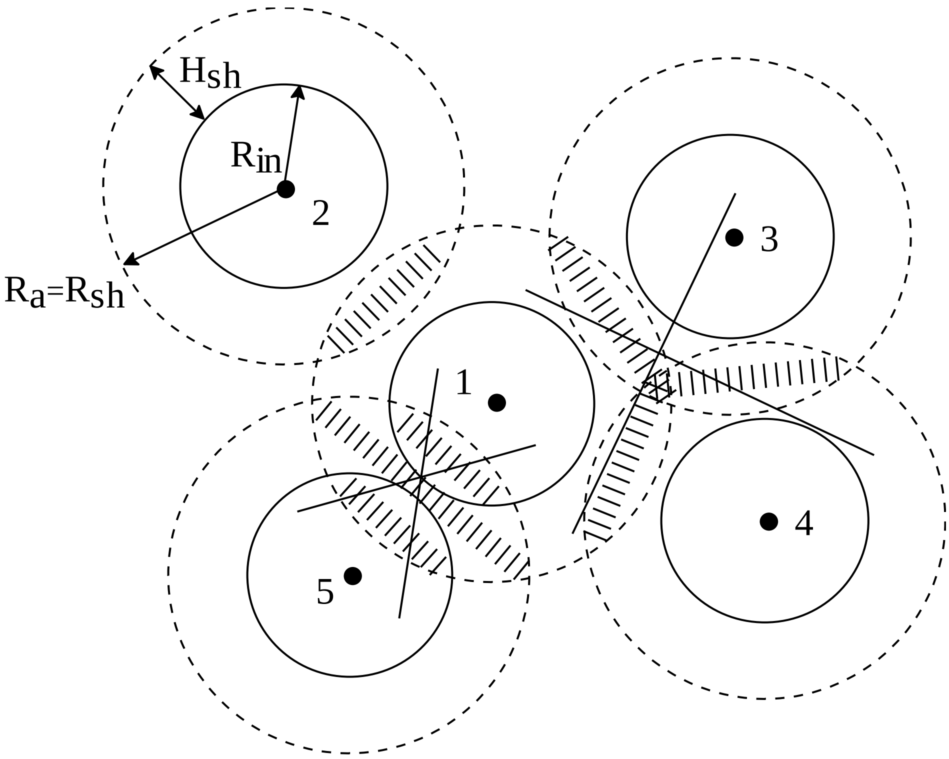

Fig. 2 Scheme of mutually penetrating atoms and the rule of pair mutual penetration during their joining. Dashed are the regions of pair mutual penetration.

If two atoms penetrate the third one, their regions of pair mutual penetration that are formed with the common for both, third, atom should not penetrate each other, in accordance with the Pauli exclusion principle (atoms 1 and 3, 1 and 4, 3 and 4 in Fig. 2).

The region of inner electrons of atom (in Fig. 2 it is bounded by a circle of solid line) is usually totally filled by electrons. Thus, other electrons, including the electrons of other atoms, cannot penetrate it also, in conformity with the Pauli exclusion principle (atoms 1 and 5 in Fig. 2).

2.3 Self-organization of atoms during mutual penetration

Atoms are electrically neutral. The inner electrons neutralize an equal number of the nuclei protons. The rest of protons is neutralized by outer electrons. For this, according to the electrostatics laws, the charge of outer electrons should be uniformly distributed over the outer sphere of the shell of outer electrons of atom.

Attractive forces between atoms can appear when their shells mutually penetrate each other, Fig.3.

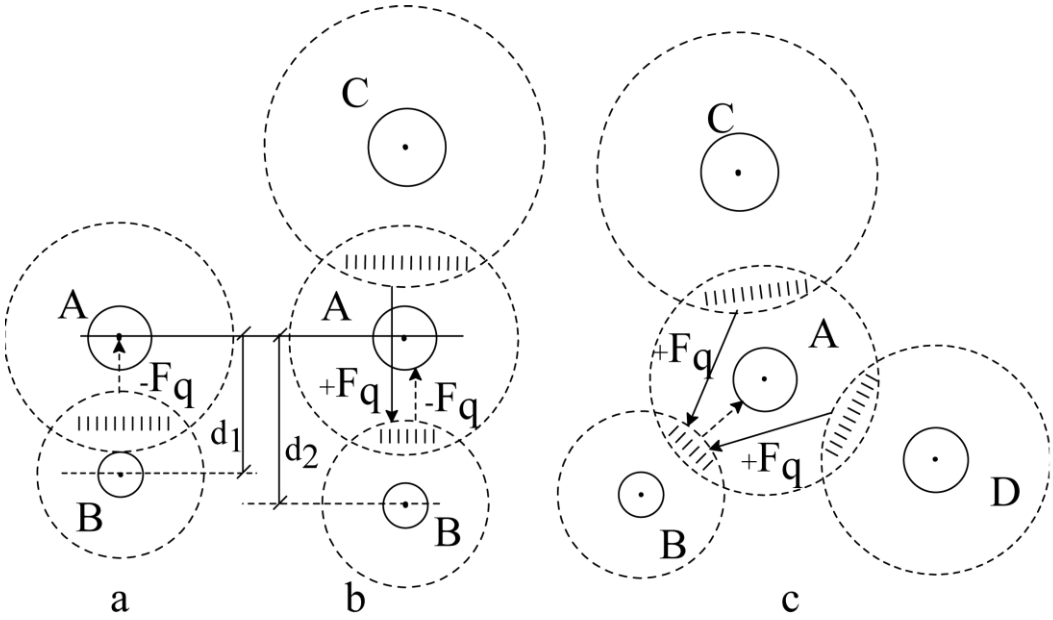

Fig. 3 Self-organization of atoms into a condensed structures. Shown are the forces acting upon the atom B (see explanation in text).

Mutually penetrated atoms attract each other by the Coulomb forces. These forces appear between the penetrated negatively-charged cupolas and positively-charged protons that are not compensated by inner electrons of the atoms in which the cupolas penetrate. Mutually penetrated atoms can approach as close as a distance d_1 (Fig.3a) at which the shell of one atom is closest to the region of inner electrons of other atom. If yet another atom penetrates (Fig.3b), a Coulomb repulsive force appears between the penetrated cupolas. The distance between the centers of the first two atoms should increase up to d_2. Due to the penetration of the third atom, the additional repulsive Coulomb forces appear which arrange atoms in a new way (Fig.3c).

So, taking into account quantum character of electrons and classical properties of atoms, one can conceive the combined quantum-classical model of atoms, their mutual penetration during packing, appearance of interatomic forces, atomic displacements, and, as a result, self-organization of atoms and formation of atomic structures [3, 4].

III Atomic mechanism of elastic deformation

Using the model of mutually penetrating atoms, we construct the cell (Fig.4) that is analogous to the cell shown in Fig.1. The cell consists of atoms A, B, C, and D which penetrate into each other with their shells. The positively charged protons of atoms (A, B, C, and D), that are not compensated by inner electrons, and the negatively charged penetrating cupolas (1A, 1B, 2B, 2C, 3D, 3C, 4A, 4D) are mutually attracting. Negatively charged cupolas penetrating the shell of the same atom mutually repulse [5, 6]. Besides, the repulsive forces are caused by thermal vibrations of atoms. The higher the temperature, the higher are the amplitude of vibrations and the distance between atoms. Distance between the atomic centers l corresponds to the equilibrium of forces of interatomic attraction and repulsion.

A tensile stress increases the distance between pairs of atoms AB and CD up to $l+d_1l$ along the axis of the applied force F. Cupolas that are perpendicular to the direction of elongation (pairs of cupolas 1A, 1B and 3D, 3C in Fig.4) decrease.

Thus, uncompensated charges of protons of atoms B and C and A and D can attract closer the cupolas that lay in the perpendicular to force F direction (pairs 2B, 2C, and 4A, 4D in Fig.4). The distances between atoms B and C, and A and D in the direction, that is perpendicular to the tensile stress, decrease (from l to $l\text{-}d_2l$ in Fig.4). So, the sample contracts in the transverse direction. Under the uniaxial compression the scheme is reverse. After releasing the stress, the Coulomb (electrostatic) forces between cupolas and atomic nuclei with participation of the thermal vibrations restore the initial sizes of the cells.

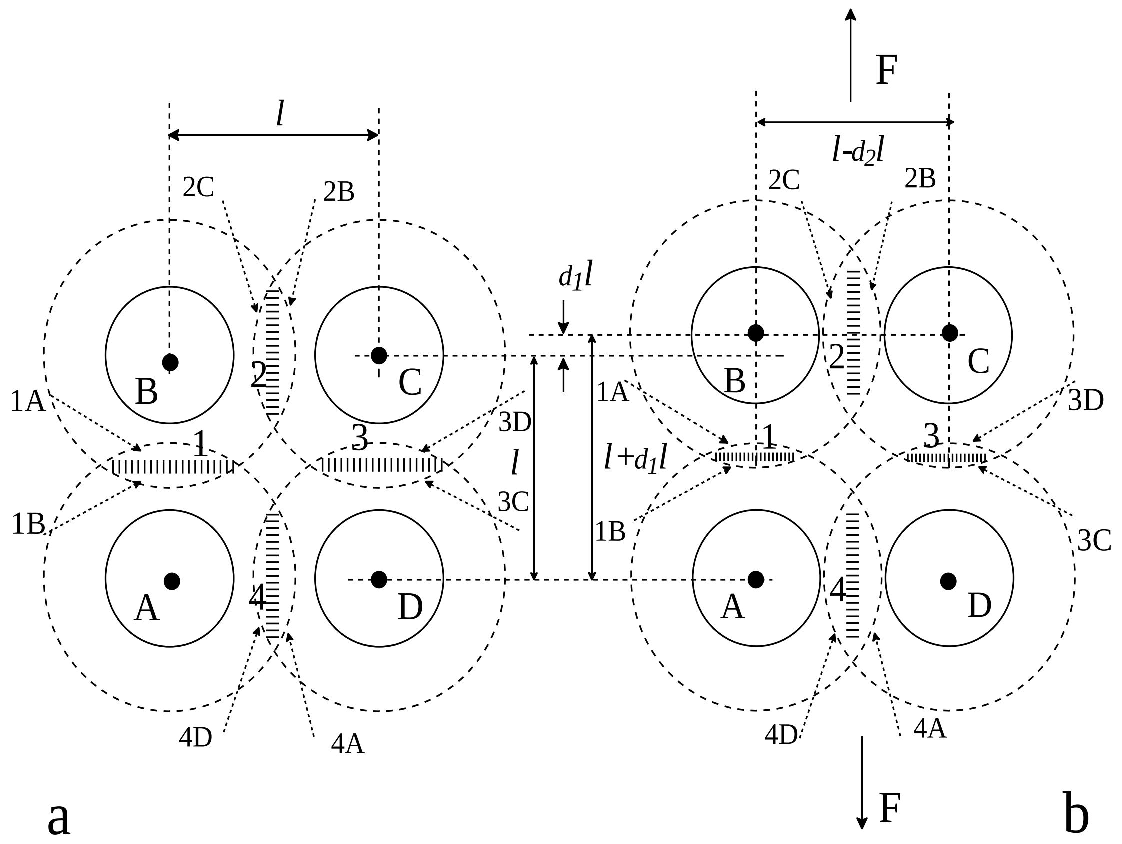

Fig. 4 Scheme of contraction of the cell under elastic tensile stress (see explanation in text)

IV Conclusion

Apparently, matter passes from its quantum form to the classical one through atoms.
Objects in quantum state are elementary particles, whose existence corresponds to the Heisenberg uncertainty principle. Substance in a classical state is objects living under the laws of classical mechanics and physics. Atoms as objects of a transitional state show quantum properties in a modified form, for example, the electrons in atom are arranged not arbitrary but in accordance with the Pauli exclusion principle. The most important classical property of an atom is the precise certainty of its position.

Elementary particles constituting atom cannot manifest only their individual properties during interaction of the atom with other atoms and outer objects and impacts, as, for example, a brick in the wall cannot manifest only its individual properties. Obviously, atom is an aggregation with new properties which are not possessed by elementary particles constituting the atom. For example, protons and electrons are particles with electric charges, while atom is a neutral particle, that is, a particle with a new quality. Even the released from atom, knocked-out, elementary particles carry traces of their previous being in the structure of atom.

The attempts to present the interaction between atoms as an interaction between their electrons are evidently incorrect. Atoms interact between each other, with environment, or some impacts not by their separate parts, but as a whole. And the atomic constituents interact with outer factors (and with inner ones) not separately, not independently, but in accord. Self-consistency of fields of charges of protons and electrons provides the electric neutrality of atom and certainty of its sizes. Inner electrons compensate the charge of the corresponding number of protons. Neutrality of atom is possible if the charge of its outer electrons is uniformly distributed over its spherical surface. Self-consistency of the charges of protons and electrons provides appearance and existence of a charge sphere of a certain size around nucleus. This is confirmed experimentally: atoms are neutral. As far as orbits and orbitals concerned, this is hypotheses.

Charge spheres are a result of a self-consistent interaction of quantum particles, and, seemingly, that is why the charge spheres have quantum properties, they tunnel, penetrate each other, and only pairwise in accordance with the quantum rules. At the same time the charge spheres have already a classical property: a certain size.

Using the arguments described above in favor of the model of interpenetrating atoms, it is possible to understand, in a rather simple way, the reason, mechanism of changing and details of behavior of the sizes of a solid body during elastic tensile and compressive stress.

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