

On Physical Nature of the Long-Range Effect during the Crystal Growth through Boundary Layers

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Abstract

A mechanism of the long-range effect in the processes of crystal growth through boundary layers based on the study of the nature of the chemical bond between the deposited and surface atoms is proposed. It is shown that the spatial distribution of the probability of finding a negative binding charge (i.e. its density) cannot be considered strictly fixed between the nearest neighboring ion cores. It also extends with decreasing quantity to other interatomic regions along the preferred directions which are determined by the electrostatic and electromagnetic fields of atomic cores and their valence electrons. The directivity and intensity of these crystalline fields are much larger than the directivity in the formed amorphous or polycrystalline layer, so they will permeate it up to some thickness. Consequently, in contrast to the clean surface where, due to the absence of atoms from the surface side, the field structure of the crystal changes, crystallographic oriented fields will penetrate to the surface of the boundary layer up to its certain thickness, which ensures the crystallinity of the deposited material.

Keywords: Long-range effect; Chemical bonds; Crystal growth; Boundary layers; Crystalline fields

Introduction

The long-range effect in crystal growth processes through amorphous or polycrystalline boundary layers consists in oriented crystallization in the of absence of a direct contact between the crystalline substrate and the deposited substance, discovered in the 1970s, which physical nature, in our opinion, has not yet been identified [1,2]. According to the generally accepted ideas, the deposited material should have an amorphous or at best a polycrystalline structure. But on the outer side of the boundary layers, single-crystal films are formed and, in most cases of better quality than grown in identical conditions on control sites, without buffer layers [3-7]. It is noted that "the transfer of the structural information does not depend on the crystallographic orientation of microcrystals" [2]. But the effect decreases with an increase in the buffer layer thickness and completely disappears at thicknesses of approximately 20 nm [1]. Today, to explain this interesting phenomenon, it is assumed: "On the surface and in the bulk of the crystal - substrate, there might be charged local active centers, representing point defects and their micro- and macro clusters, which causes the emergence of an induced polarization structure in the diffraction-amorphous boundary layers that can transmit and "store" the structural information. The active charged centers located in the bulk and on the surface can form polarization-charged bridges capable of transmitting the structural information over significant distances through the buffer layers", which has not been experimentally proved [2]. Here, an assumption is made: "In the amorphous boundary layers, a short-range order may exist – a "single-crystal" electric order sufficiently independent of the atomic structure of the layers" [2]. But the detection of information properties of the boundary metal layers which, according to the accepted notions, shorting the electrically active centers, completely shield the potential relief of the surface of solids and should not have any information properties, impelled the authors to make another controversial, in our opinion, assumption: "In the boundary layers near the active metal centers of the crystal surface - substrate, local semiconductor and/or dielectric metal compounds are formed where electret-type polarization microstructures are induced" [2].

Results and Discussion

In this paper, we propose a mechanism of the long-range effect in crystal growth processes through boundary layers, based on the consideration of the nature of the chemical bond between the deposited and surface atoms and its variation depending on the conditions of their interaction in the deposition process. As is known, the nature of the chemical bond, despite significant advances

in quantum chemistry, has not been fully established [8]. There are several approaches to the solution of this problem, and all of them are based on the assertion that the chemical bond is realized by electrons between the ion cores of the corresponding atoms [9-11]. It is believed that "the real bond in chemical compounds is intermediate between ionic, covalent and metallic bonds" [8]. It is known that in molecules consisting of different atoms, the negative charge density of the bonding electrons is shifted towards the atom with a higher electronegativity (EN), i.e. a polarization of the chemical bond takes place [8]. But, since "EN is not a strict physical quantity that can be directly determined experimentally, is not constant and depends on the nature of the other atom with which the given atom is chemically bound", in order to estimate the fields of ion cores that determine the density distribution of the negative charge of binding electrons, we decided to use a completely determined constant value - the specific bonding energy of valence electrons with their ion cores, calculated from

$$\bar{I} = \frac{\sum_{i=1}^n I_i}{n} \quad (1)$$

where I_i is the ionization energy of the i^{th} valence electron, obtained, however, not by non-sequential ionization of atoms, but by ionization of the neutral atom for each of the n -valence electrons [12,13]. In contrast to the covalent bond, the electrostatic interaction of the unlike charges is not subject to saturation [8]. If the negative charge is attracted to one positive charge, this by no means prevents it from being attracted simultaneously to other positive charges. This explains the apparent contradiction that when passing from gaseous molecules to crystals, a noticeable increase in the bond length is observed, accompanied, nevertheless, by bond strengthening. Despite the fact that each individual bond in the crystal is weaker than in the relevant molecule, the number of bonds with other atoms is much larger, which increases the total interaction energy [12]. Naturally, with increasing distance from the atomic core to which the valence electron belonged, the interaction force will decrease due to the screening by electrons and ion cores. Thus, the spatial distribution of the probability of finding a negative charge (i.e. its density) cannot be considered strictly fixed between the nearest neighboring ion cores, it will also extend to other interatomic regions* in the preferred directions that are determined by electrostatic and electromagnetic fields of atomic cores and their valence electrons. To characterize the intensity of this extension, it is probably possible to use the specific bonding energy of valence electrons, since the larger its value, the better the preservation of the directivity and intensity of the fields that determine the chemical bonds. Proceeding from the above, a crystalline body can be represented as a field structure of a set of electrostatic and electromagnetic fields with clearly defined directions and magnitudes. This idea was first expressed by E. Schrödinger: "I rather consider the whole structure of the crystal lattice as something very related to the de Broglie standing wave. ... Then the entire process of interaction can be represented as an interaction of the field structures or wave functions. On this path, however, enormous difficulties may arise, ... and one has to resort to "chemical and mathematical intuition" and engage in "guesswork" [16,17]. From the works of the discoverers of the effect under discussion - G.I. Distler and his collaborators [3,4,6,18,19,20], it follows that "the effective active surface of a solid body is as if elevated at some distance from its geometric surface" [2]. To explain this assumption, we consider the directivity of the fields on the surface of the crystalline body before and after deposition of the intermediate layer. The absence of atoms from the surface side, which were supposed to attract electrons participating in the creation of the chemical bond, changes the directivity of the crystal fields, and these electrons are attracted by neighboring surface and subsurface atomic cores. There is a flow of the charge

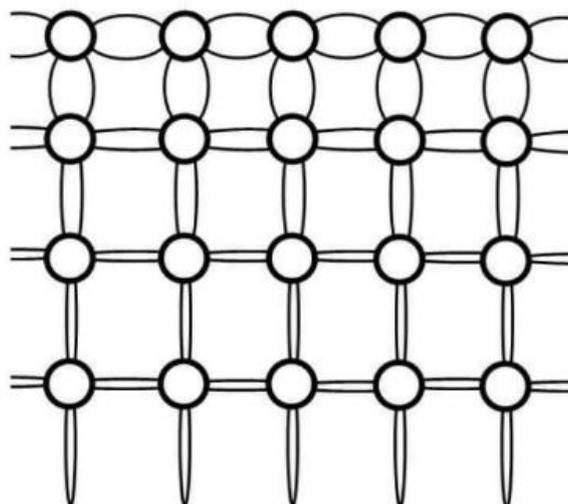


Figure 1: Schematic representation of the flow of the excessive density of the binding negative charge to the chemical bonds of atoms located on and in the bulk of the sample

* Such a dynamic approach is used in the description of the electrometric and inductive effects, despite the fact that the quantitative estimates are not sufficiently well defined [14,15].

density of the bonding electrons over the surface and into the bulk of the crystalline body (Figure 1), which accordingly increases the strength of the chemical bond. This explains the increase in the surface hardness of solids [21,22] (Figure 2). Thus, the surface region, as rightly noted in, can be regarded as a special phase with completely different characteristics than the volume phase and extending into the bulk of the solid [2,23]. For different substances, the penetration of this excess density of the binding charge into the bulk of the solid will be the higher, the higher the specific bonding energy of the valence electrons with their ion cores, and the smaller the dielectric constant (Figure 2) [24]. This depth can be approximately estimated by a decrease in the microhardness with increasing penetration depth of the indenter. The flow of the charge density of the binding electrons changes the field structure of the crystal in the sense that the fields do not due to their interaction with the surface atoms, the gradual reverse flow

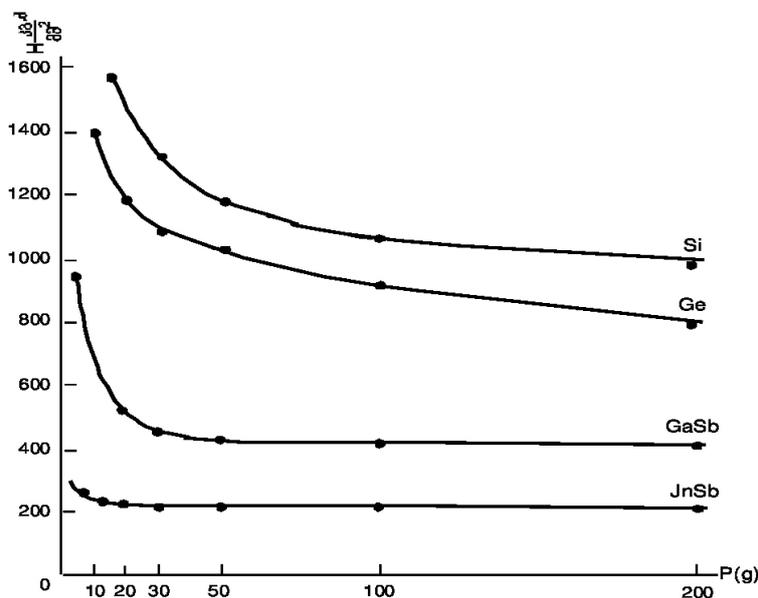


Figure 2: Dependence of the microhardness H of the substance on the load P (g) on the indenter (the higher the load, the greater penetration depth of the indenter)

of the charge density of the binding electrons and the restoration of crystal fields with the directivity and intensity much larger than the directivity in the formed amorphous or polycrystalline layer take place. Naturally, these fields will decrease due to the screening by other electrons and ion cores of the boundary layer, but they will still permeate it up to some thickness. Consequently, on the surface of the boundary layer, up to certain thicknesses, in contrast to the clean surface, crystallographic oriented fields will extend, which ensures the crystallinity of the deposited material. It is the gradual reverse flow of the charge density of the bonding electrons and the restoration of crystalline fields that explains the "paradoxical, at first sight, phenomenon which consists in improvement of the degree of orientation of the layers deposited in vacuum as their thickness increases" [2]. The change in the quality of the long-range effect as a result of various external actions (gamma-ray irradiation, chemical or ion etching, the impact of various fields) is due to the fact that they change the field structure of the surface layer of the crystal [2,25].

Thus, the field structure of the crystal lattice consisting of a set of electrostatic and electromagnetic fields that permeates the boundary layers to a certain thickness is a crystallographic orienting field that ensures the crystallinity of the deposited layer.

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