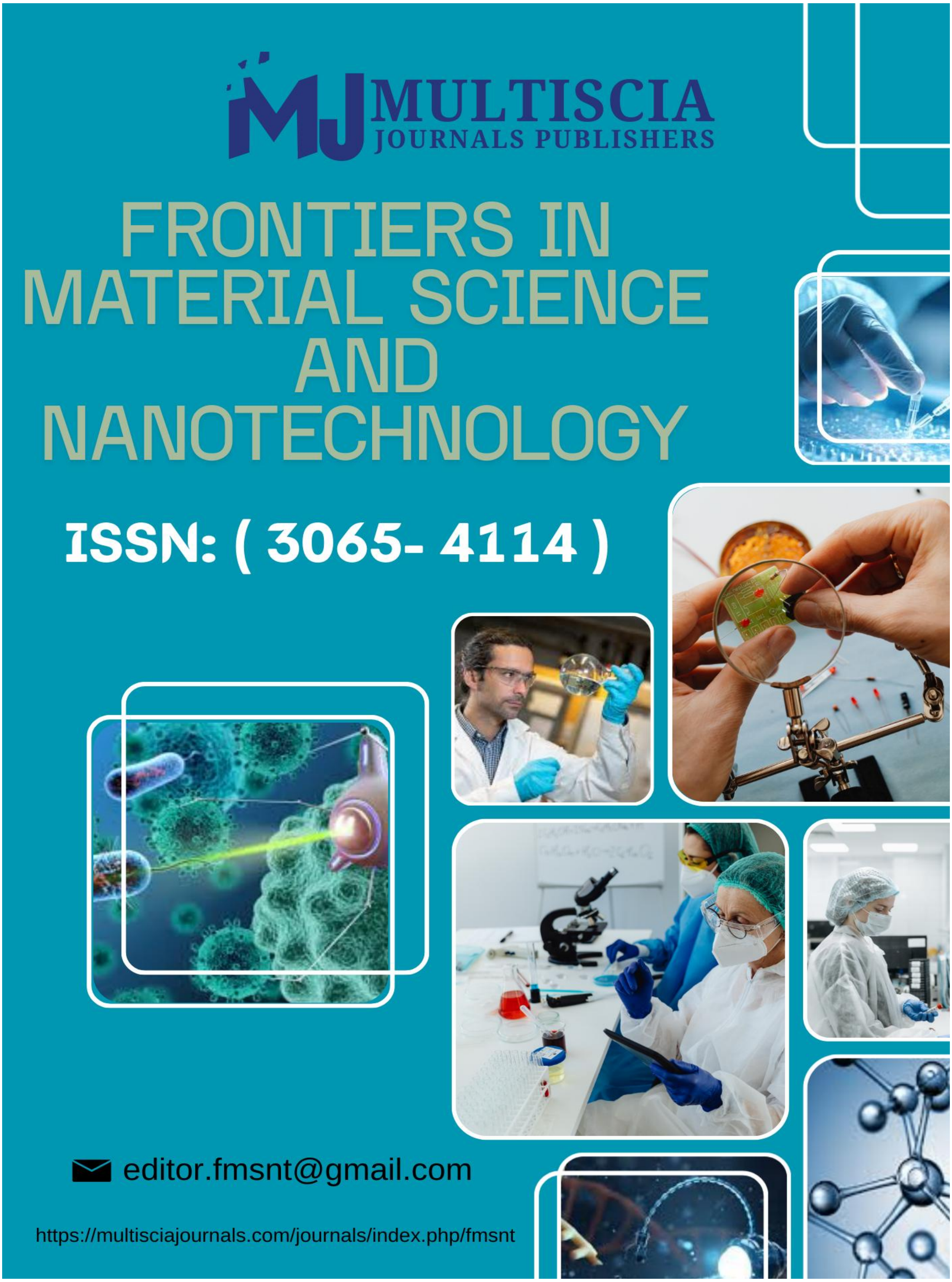

MJ MULTISCIA
JOURNALS PUBLISHERS

FRONTIERS IN MATERIAL SCIENCE AND NANOTECHNOLOGY

ISSN: (3065- 4114)

editor.fmsnt@gmail.com

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Frontiers in Material Science and Nanotechnology
Volume1, Issue1, 2025

Regarding the Quantum Character of the Long-Range Impact on Crystal Growth via Boundary Layers

Bcuachidze Y[1], and Meftonidze R[2]

[1]Department of **Material Science and Nanotechnology**

Article Info

Received: 30-01-2025 ***Revised:08-03-2025*** ***Accepted:18-03-2025*** ***Published:29-03-2025***

Abstract

Based on research into the chemical link between deposited and surface atoms, a model for the long-range influence in crystal formation processes via boundary layers is put forth. The distribution of the density, or likelihood of finding a negative binding charge, cannot be regarded rigidly stable between the closest nearby ion cores, as shown. The favored routes, dictated by the electrostatic and electromagnetic fields of atomic cores and their valence electrons, also extend to other interatomic regions, but in diminishing quantities. These crystalline fields will penetrate the generated amorphous or polycrystalline layer to a certain thickness due to their much higher directivity and intensity compared to the layer's own directivity. Crystallographically oriented fields will penetrate the surface of the boundary layer up to a certain thickness, ensuring the crystallinity of the deposited material, in contrast to a clean surface where the field structure of the crystal changes due to the absence of atoms from the surface side.

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

Introduction

We still don't know the physical nature of the long-range effect identified in the 1970s—oriented crystallization in the absence of direct contact between the crystalline substrate and the deposited substance—that occurs in crystal growth processes through amorphous or polycrystalline boundary layers [1,2]. Our current best guess is that the deposited material will be either completely amorphous or very slightly polycrystalline. However, single-crystal films are created on the boundary layers' outer surfaces, and these films are often of higher quality than those developed on control sites without buffer layers under the same circumstances [3-7]. It's important to highlight "the transfer of the structural information does not depend on the crystallographic orientation of microcrystals" [2]. The impact, however, diminishes as the buffer layer thickness rises and vanishes altogether at around 20 nm thicknesses [1]. A current working hypothesis attempts to shed light on this intriguing phenomenon by positing the following: "In the bulk of the crystal-substrate and on the surface, there may be charged local active centers representing point defects and their micro- and macro clusters. This leads to the formation of an induced polarization structure in the diffraction-amorphous boundary layers, which can transmit and "store" the structural information. An unproven theory states that "polarization-charged bridges formed by active charged centers in the bulk and on the surface can transmit the structural information over significant distances through the buffer layers" [2]. "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]. This order is assumed to exist in the boundary layers. We find the authors' assertion that "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] to be highly problematic, as it leads them to assume that boundary metal layers—which, according to conventional wisdom, completely shield the potential relief of solid surfaces—should not have any information properties.

Results and Discussion

Given the nature of the chemical bond between the deposited and surface atoms and how it changes depending on the conditions of their interaction during deposition, we present a mechanism for the long-range effect in crystal growth processes through boundary layers in this paper. It is well-established that, notwithstanding notable advancements, the chemical link remains fundamental.

in the field of quantum chemistry, is still up for debate [8]. Electrons between the ion cores of the matching atoms realize the chemical connection, according to many methods that aim to solve this difficulty [9–11]. According to experts, "the real bond in chemical compounds is intermediate between ionic, covalent and metallic bonds" [8]. It is well-known that when different atoms in a molecule are bonded, the electrons' negative charge density is moved to the atom with a greater electronegativity (EN), a process known as polarization of the chemical bond [8]. However, due to the fact that "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," we opted to utilize a fixed value—the specific bonding energy of valence electrons with their ion cores, computed from

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

where Ii is the ionization energy of the i th valence electron, which is calculated by ionizing the neutral atom for each of the n-valence electrons rather than by non-sequential ionization of atoms [12,13]. The saturation of the electrostatic interaction between dissimilar charges does not occur in covalent bonds [8]. Just because a negative charge is drawn to one positive charge doesn't imply it can't be drawn to other positive charges at the same time. In this way, the seeming paradox of link strengthening occurring simultaneously with a discernible increase in bond length when molecules transition from gas to crystals is explained. The overall interaction energy is higher in a crystal because there are more bonds with other atoms, even if the strength of each bond is lower than in the corresponding molecule [12]. The screening effect of electrons and ion cores causes the interaction force to diminish as one moves away from the atomic core that the valence electron originally belonged to. This means that the density of negative charges, as a function of space, is not limited to the immediate vicinity of neighboring ion cores but rather extends to other interatomic regions* along the preferred axes defined by the electrostatic and electromagnetic fields of the atomic nuclei and their valence electrons. It is likely that the specific bonding energy of valence electrons may be used to assess the strength of this extension, because a bigger value provides better preservation of the directivity and intensity of the fields that govern the chemical bonds. From the above, we may deduce that a crystalline body is best described as a field structure consisting of a collection of well-defined electrostatic and electromagnetic fields. "I prefer to think of the entire crystal lattice structure as something very related to the de Broglie standing wave," E. Schrödinger first stated this theory. By doing so, we may depict the whole interaction process as an interplay of field structures or wave functions. However, one may face significant challenges along this journey and have to rely on "chemical and mathematical intuition" and "guesswork" [16,17]. "The effective active surface of a solid body is as if elevated at some distance from its geometric surface" [2] is the reasonable conclusion to draw from the research of G.I. Distler and colleagues, who discovered the phenomenon in question [3,4,6,18,19,20]. In order to clarify this presumption, we look at the field directivity on the crystalline body's surface both before and after the intermediate layer is deposited. In the chemical bonding process, atoms on the surface were expected to attract electrons. However, when these atoms are absent, the crystal fields become less directed, and instead, electrons are drawn to nearby surface and subsurface atomic cores. The charge is moving through a system.

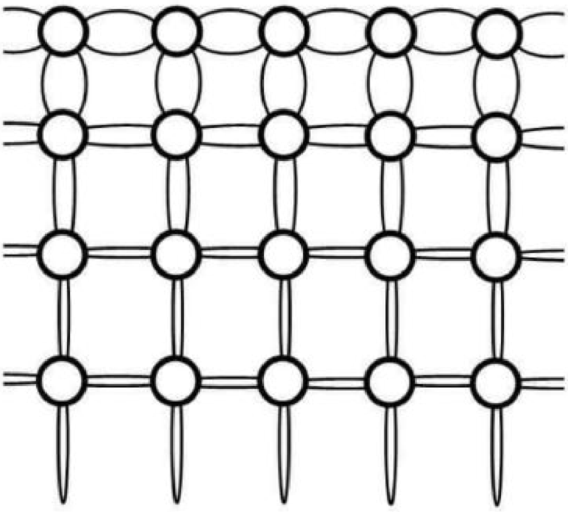

Figure 1: Schematic representation of the flow of the excessive density of the binding negative charge to the chemical bonds of atoms located on and in the bulk of the sample

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

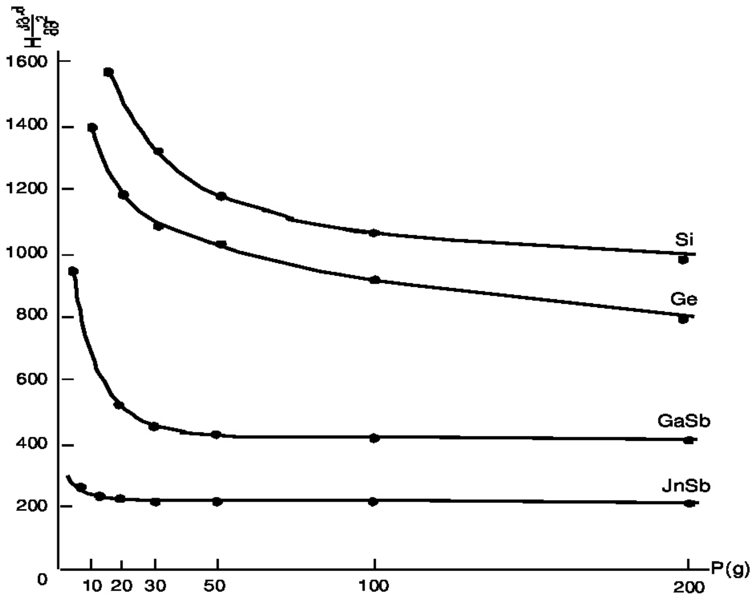

Figure 2: Dependence of the microhardness H of the substance on the load P (g) on the indenter (the higher the load, the greater penetration depth of the indenter)

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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