

Molecular Dynamics Analysis of Atomic Diffusion and Crystallization Behavior of Pure Silver in the Vitreous State under Varied External Pressures

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SPECIAL ISSUE ON:

The 2024 1st International Conference
on Materials Sciences and Mechatronics
for Sustainable Energy and the Environment
October 1-3, 2024 at Béni-Mellal, Morocco

KEYWORDS

Molecular dynamics; Silver
metallic glass; Atomic
diffusion; Crystallization;
External pressure; Vitreous
state.

ABSTRACT

This study investigates the atomic diffusion and crystallization behaviour of pure silver in the vitreous state under varying external pressures, using molecular dynamics simulations. The primary aim is to assess the effects of pressure on the structural dynamics and stability of silver at the atomic level. The results indicate that increasing pressure leads to a decrease in diffusion coefficients, signifying reduced atomic mobility due to denser atomic packing. Structural analysis through Voronoi tessellation reveals a shift from distorted, mixed-like clusters toward a predominance of crystal-like clusters, suggesting enhanced crystallinity with higher pressures. This is further supported by an increased frequency of 14-coordinated clusters in the coordination number distribution. These findings highlight the impact of pressure on the structural ordering of metallic glass and offer insights into its behaviour at different length scales.

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تحليل الديناميكيات الجزيئية لانتشار الذرات وسلوك التبلور للفضة الخالصة في الحالة الزجاجية تحت تأثير ضغوط خارجية متغيرة

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ملخص: تتناول هذه الدراسة انتشار الذرات وسلوك التبلور للفضة الخالصة في الحالة الزجاجية تحت تأثير ضغوط خارجية متغيرة باستخدام محاكاة الديناميكيات الجزيئية. الهدف الأساسي هو تقييم تأثير الضغط على الديناميكيات الهيكلية واستقرار الفضة على المستوى الذري. أظهرت النتائج أن زيادة الضغط تؤدي إلى انخفاض في معاملات الانتشار، مما يدل على انخفاض حركة الذرات بسبب زيادة كثافة التعبئة الذرية. وكشفت التحليلات الهيكلية باستخدام تقسيم فورونوي عن تحول من تجمعات مشوهة ومختلطة إلى هيمنة التجمعات البلورية، مما يشير إلى تعزيز التبلور مع ارتفاع الضغوط. وتؤكد هذه النتائج زيادة تكرار التجمعات ذات التنسيق الرباعي عشر في توزيع أعداد التنسيق. تسلسل هذه النتائج الضوء على تأثير الضغط على الترتيب الهيكلي للزجاج المعدني وتوفر رؤى حول سلوكه على مستويات طول مختلفة.

الكلمات المفتاحية – الديناميكيات الجزيئية، الزجاج المعدني، انتشار الذرات، التبلور، الضغط الخارجي، الحالة الزجاجية.

1. INTRODUCTION

Metallic glasses, also known as amorphous metals, represent a unique class of materials characterized by their lack of long-range atomic order, distinguishing them from traditional crystalline metals. These materials are typically formed through the rapid cooling of a liquid alloy, which prevents the atoms from organizing into a regular crystalline structure [1-3]. This disordered arrangement imparts metallic glasses with exceptional mechanical and physical properties, such as high strength, excellent corrosion resistance, and superior elastic limits, making them valuable for a wide array of applications [4,5].

In this study, pure silver is selected as the system of interest due to its well-documented atomic structure and diffusion characteristics. Silver's simple composition and high atomic diffusivity make it an ideal candidate for investigating the fundamental behaviors of metallic glasses under various conditions. This focus allows for clearer insights into the mechanisms governing metallic glass behavior without the complexities introduced by alloying elements [6-9]. Recent studies have highlighted the promising potential of metallic glasses in various applications, particularly in the fields of energy storage and conversion. For instance, Ding et al. demonstrated that the amorphous structure of metallic glasses can significantly enhance their electrochemical performance, enabling faster charge and discharge cycles in battery applications [10]. Similarly, Hasannaemi et al. investigated the use of metallic glasses in hydrogen fuel cells, emphasizing their mechanical stability under operational stress [11]. The guiding question for this investigation is: How does external pressure influence the dynamic and structural properties of silver metallic glass? Understanding these properties is crucial for predicting the performance of metallic glasses in practical applications.

Despite advancements in recognizing the potential of metallic glasses, the influence of external pressure on their dynamic and structural properties remains inadequately explored. While some research has focused on how pressure affects the mechanical properties of these materials, the underlying atomic mechanisms driving these changes are still not well understood. Most existing studies, such as those by Hu et al., primarily address high-pressure behavior but do not comprehensively analyze the interplay between pressure, atomic mobility, and structural changes [12]. The increasing demand for efficient energy storage and conversion technologies necessitates the development of advanced materials that can withstand varying operational conditions while maintaining optimal performance. Metallic glasses, including silver metallic glass, exhibit promising attributes for these applications due to their unique structural properties,

which can enhance ionic and electronic transport mechanisms crucial for energy storage devices. For instance, the amorphous nature of metallic glasses can lead to improved electrochemical performance, enabling faster charge/discharge cycles and higher energy densities, thereby addressing the limitations of conventional crystalline materials [13]. Furthermore, the ability of metallic glasses to maintain structural integrity under mechanical stress enhances their durability in energy conversion systems. This characteristic promotes long-term stability and reliability in applications such as hydrogen fuel cells and solid-state batteries, where mechanical stability is paramount [11].

To thoroughly explore these properties, molecular dynamics (MD) simulations are employed in this research. MD simulations provide a powerful tool for studying materials at an atomic level, offering detailed insights into the behavior of metallic glasses that are often difficult to observe experimentally [14]. By simulating the system under controlled conditions - including changes in pressure and temperature - researchers can systematically examine how these factors influence the dynamic and structural characteristics of silver metallic glass. This approach not only enhances our understanding of the atomic-scale mechanisms at play but also aids in the design and development of new materials with tailored properties suitable for advanced applications. The organization of this paper is outlined as follows: Section 2 describes the simulation methods and computational details; Section 3 provides the results and discusses the findings related to the dynamic and microstructural properties of the silver metallic glass; and finally, Section 4 summarizes the main conclusions, highlighting the significant insights and suggesting directions for future research.

2. COMPUTATIONAL DETAILS

The classical molecular dynamics software LAMMPS [15] is utilized to perform the simulations in this study, aiming to investigate how varying pressure affects the dynamic and microstructural properties of pure silver metallic glass. The simulations begin with 32,000 silver atoms arranged in a face-centered cubic (fcc) lattice structure within a cubic simulation box. Periodic boundary conditions are applied in all directions to emulate an infinite system. The interactions between the silver atoms are modeled using the Embedded Atom Model (EAM) [16], which defines the potential energy function. This model calculates the energy by considering both atomic interactions and the surrounding electron density, as detailed in the following relation.

$$E = \frac{1}{2} \sum_{i,j, i \neq j} \theta_{ij}(r_{ij}) + \sum_i F_i(\rho_i) \quad (1)$$

The embedding energy of an atom i , labeled as F_i , is influenced by the atomic electron density ρ_i , whereas θ_{ij} denotes the energy associated with interactions between pairs of atoms.

The integration of the equations of motion is performed using the velocity Verlet algorithm with a time step of 1 femtosecond (fs). Temperature control is achieved through a Nose-Hoover thermostat [17], while pressure is managed using the Andersen method [18]. The simulation initiates by increasing the temperature of a silver crystal from 300 K to 3000 K, significantly above its melting point of approximately 1235 K, at a rate of 5×10^{12} K/s within an NPT ensemble at zero pressure. Following this heating phase, the system equilibrates in the liquid state for 100 picoseconds (ps) under an NVT ensemble. To attain a glassy state, the system is then rapidly cooled from 3000 K to 300 K within the NPT ensemble, with pressures varying between 0 and 70 GPa. This cooling process is conducted at a constant rate of 5×10^{12} K/s to maintain consistent conditions throughout.

3. RESULTS AND DISCUSSION

This section delves into the dynamic and structural characteristics of silver in its glassy state under varying external hydrostatic pressures. By examining these properties across different pressure levels, we gain crucial insights into the material's behavior, establishing a fundamental understanding of its response across different length scales.

To explore the atomic-scale behavior and diffusion processes of pure silver in its glassy state under different pressures, we analyze the evolution of mean-square displacement (MSD) over time. This is calculated using the formula based from the Einstein relation [9]:

$$D = \lim_{t \rightarrow \infty} \frac{1}{6t} \langle \Delta r^2(t) \rangle \quad (2)$$

Here, t represents time, and the mean square displacement (MSD), denoted as $\langle \Delta r^2(t) \rangle$, is defined as follows:

$$\langle \Delta r^2(t) \rangle = \frac{1}{N} \left\langle \sum_{i=1}^N [r_i(t) - r_i(0)]^2 \right\rangle \quad (3)$$

Here, N denotes the total number of atoms in the simulation box. The position of particle i at time t is represented as $r_i(t)$, with $r_i(0)$ being its initial position. The symbol $\langle \dots \rangle$ indicates the ensemble average across various configurations. Fig. 1 demonstrates that, during isothermal compression at ambient temperature, the mean square displacement curves reflect a transition in atomic motion through distinct regimes ballistic, localized, and diffusive. This progression corresponds to increasing resistance against atomic displacement as external pressure grows. The ballistic regime, characterized by a t^2 relationship in MSD, implies that atoms initially move without restriction from neighboring atoms. This phase, minimally impacted by pressure due to the short timescale, reflects atomic movement that remains largely inertial and independent of interatomic forces.

As pressure increases, the emergence of extended plateaus in the MSD indicates the 'cage effect,' where atoms become temporarily trapped in local energy wells formed by their neighbors. The lengthening of this plateau with pressure suggests that atoms require higher activation energy to escape these 'cages,' with configurational adjustments becoming more constrained. This effect can be attributed to increased atomic packing density and tighter spatial restrictions, creating a scenario where atoms are dynamically hindered, reflecting a transition to localized movement. These findings correlate with prior studies on glassy materials, where enhanced pressure stabilizes the local atomic arrangements, thereby increasing the energy barriers for diffusion [19,20].

In Fig. 2, the trend of decreasing diffusion coefficients with increased pressure further illustrates this dynamic restriction. High pressures intensify the density of the atomic structure in silver metallic glass, leading to reduced free volume and restricted pathways for atomic migration. This trend highlights the impact of structural densification on atomic mobility, where less accessible space within the glassy matrix restricts atomic rearrangement. Under these conditions, the system exhibits a slowed kinetic response and a tendency towards a more amorphous, structurally compact state. This observation aligns with the fundamental concept of pressure-induced densification in metallic glasses, which is known to hinder long-range atomic diffusion due to limited interstitial spaces.

Overall, the distinct MSD behavior and the reduction in diffusion coefficients provide insights into the interaction between atomic movement and the microstructural evolution of silver metallic glass under high-pressure conditions. As pressure intensifies, atomic movement transitions from ballistic independence to caged localization and finally to constrained diffusion, suggesting that hydrostatic pressure not only affects atomic diffusion but also reinforces structural stability and

density in the glassy state. These results shed light on how pressure-modulated environments can be used to tune the mechanical and structural properties of metallic glasses, which is crucial for applications requiring materials with tailored durability and low atomic mobility.

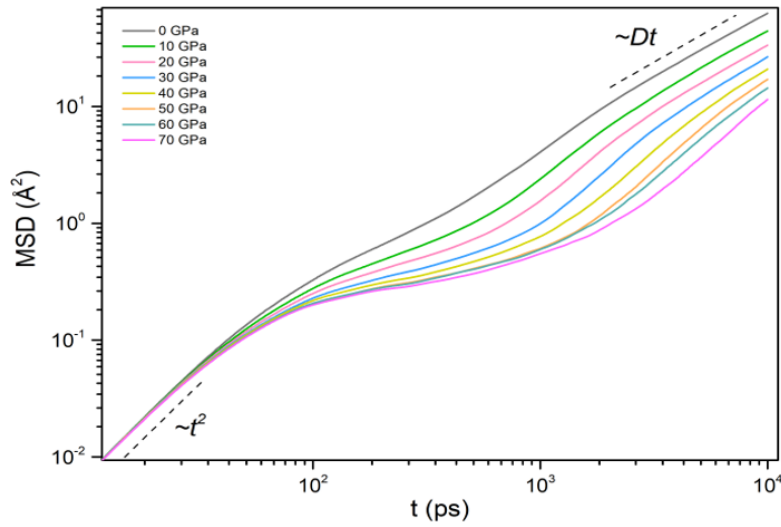


Fig. 1. Mean-square displacement dynamics of pure silver in the glassy state under isothermal compression at various pressures.

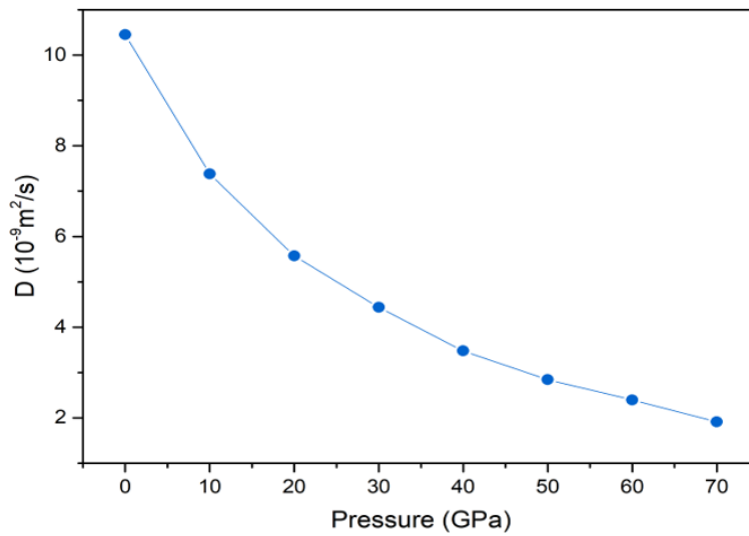


Fig. 2. Diffusion coefficients of silver metallic glass as a function of isothermal pressure.

To examine the structural tendencies of silver in its glassy state under varying pressures after the glass transition, we initially conducted an analysis of the pair distribution function (PDF) across different compression levels, ranging from 0 to 70 GPa. The PDF measures the probability of locating a particle at a given distance from a reference particle within the material. It is expressed as [21]:

$$g(r_i) = \frac{V}{N^2} \left\langle \sum_{j \neq i}^N \frac{n(r_i)}{4\pi r_i^2 \Delta r_i} \right\rangle \quad (4)$$

Here, V is the system's volume, N is the total number of atoms, and $n(r)$ represents the number of neighbouring atoms within a radial distance from r to $r+\Delta r$ around a reference atom. The PDF provides insights into the atomic arrangement and local structure of materials, helping to identify patterns in liquids, glasses, and crystalline solids [22].

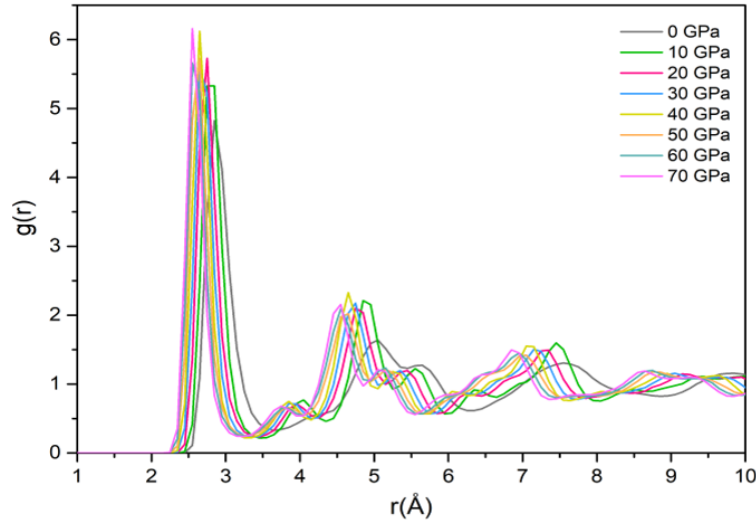


Figure 3. PDF of silver at 300 K under varied pressures ranging from 0 to 70 GPa with a quenching rate of 5×10^{12} K/s.

Fig. 3 illustrates the significant changes in the radial distribution function $g(r)$ as pressure increases, reflecting profound alterations in atomic arrangements within silver metallic glass. The movement of peaks toward smaller distances r indicates a reduction in nearest interatomic distances, suggesting that atoms are compressed into closer proximity. This densification reduces free volume and enhances local atomic ordering, as evidenced by the increased heights of the peaks. Notably, the splitting of the second peak into two distinct sub-peaks signifies an enhancement in medium-range order, indicating a transition toward more organized, crystalline-like structures. This behavior aligns with the typical pressure-induced densification phenomena observed in metallic glasses, where increased atomic packing results in a more stable configuration [22]. Furthermore, the enhanced local order at elevated pressures suggests a promotion of crystallization within the material, as atoms adopt more energetically favorable arrangements that resemble those of crystalline phases, reinforcing the role of pressure in achieving a more stable structure.

To examine the local environments around each atom in the glassy state and understand how microstructural properties relate to applied pressure, we employed the Voronoi tessellation method [23]. This approach involves using the Voronoi index $\langle n_3, n_4, n_5, n_6 \rangle$ to define the Voronoi polyhedron (VP) for each atom. In this context, each n_i denotes the number of faces with i -edges that constitute the surface of the Voronoi polyhedron surrounding the central atom. Fig. 4 illustrates the changes in the most prevalent Voronoi polyhedra (VPs) during the compression and cooling process of supercooled pure silver melt. The primary VPs identified include $\langle 0, 2, 8, 4 \rangle$ (distorted icosahedral-like clusters), $\langle 0, 3, 6, 4 \rangle$ (mixed-like clusters), and $\langle 0, 4, 4, 6 \rangle$ (crystal-like clusters). The analysis shows that as pressure increases during the quenching process, the fraction of $\langle 0, 4, 4, 6 \rangle$ polyhedra rises, indicating a shift toward a greater prevalence of crystal-like structures within the metallic glass. Conversely, the fractions of $\langle 0, 2, 8, 4 \rangle$ and $\langle 0, 3, 6, 4 \rangle$ polyhedra decline, highlighting a transition from less ordered atomic configurations to more organized structures. This trend suggests that higher pressures facilitate atomic rearrangements favoring lower-energy configurations characteristic of crystalline materials, enhancing the stability and potential performance of the metallic glass [24,25]. This is evident in Fig. 5, where the distribution of central atoms within the $\langle 0, 4, 4, 6 \rangle$, $\langle 0, 3, 6, 4 \rangle$, and $\langle 0, 2, 8, 4 \rangle$ VPs is displayed. The snapshots reveal a significant transformation in the atomic structure, with crystal-like clusters becoming increasingly dominant, while distorted icosahedral-like and mixed-like clusters decline. This suggests that increased pressure promotes greater crystal ordering, thereby enhancing the short-range order within the glassy silver system.

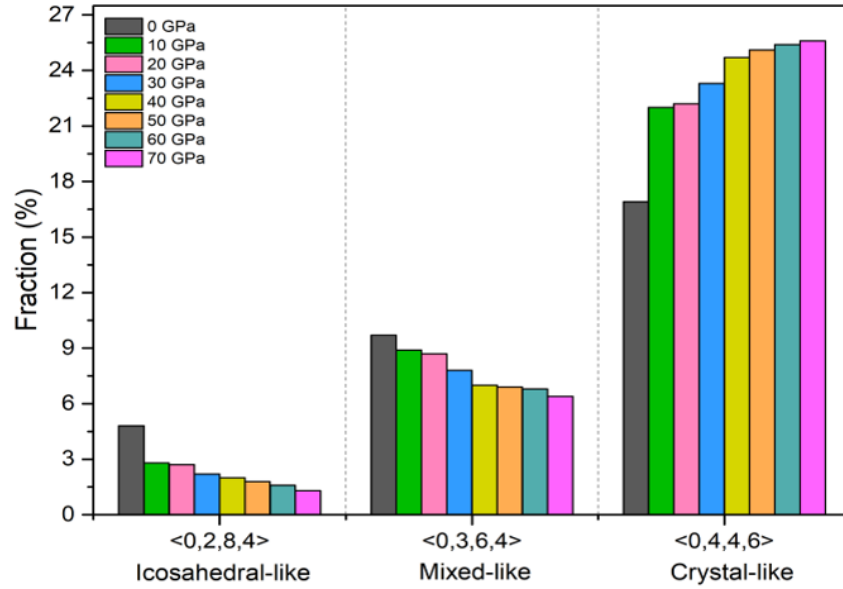


Fig. 4. Distribution of predominant polyhedra representing icosahedral-like, mixed-like, and crystal-like clusters in monatomic Ag metallic glass at different pressure conditions.

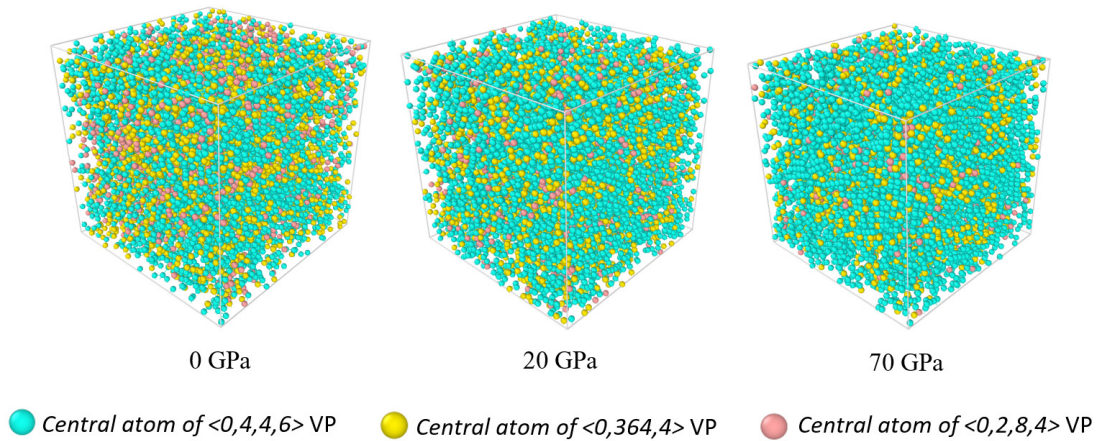


Fig. 5. Simulation snapshot of central atom distribution in <0,4,4,6>, <0,3,6,4>, and <0,2,8,4> Voronoi polyhedra in silver at ambient temperature under various pressures.

The coordination number (CN) of an atom, reflecting the count of its closest neighbouring atoms, is calculated by adding up the faces of the Voronoi polyhedron associated with that atom. This approach involves determining CN by summing the faces of the polyhedron that are directly connected to the atom. Fig. 6 displays how coordination numbers are distributed in silver metallic glass at 300 K across a range of pressures from 0 to 70 GPa, providing insights into the material's structural evolution under varying conditions. As pressure increases, the frequencies of coordination numbers 12, 13, 15, and 16 decline, while the occurrence of coordination number 14 rises significantly. This shift indicates a substantial transformation in the atomic structure, with the increasing prevalence of 14-coordinated clusters reflecting a transition towards a more ordered, crystalline arrangement. At lower pressures, the system exhibits a disordered, amorphous structure characterized by a broad range of coordination numbers, which is typical for metallic glasses where atoms occupy random positions. However, with increasing pressure, the distribution narrows, favoring the formation of 14-coordinated clusters. This trend highlights that elevated pressure enhances atomic packing efficiency, resulting in a more uniform arrangement characteristic of crystalline materials. The rise in 14-coordinated clusters suggests that pressure facilitates atomic rearrangements that reduce free volume and strengthen attractive interactions

between neighboring atoms. Thus, this enhanced packing contributes to a more structured state within the metallic glass. Overall, this analysis of pressure's impact on local atomic environments in silver metallic glass elucidates fundamental principles governing its behavior and emphasizes the role of pressure in influencing structural ordering.

To closely examine the distributions of coordination numbers in the simulated silver system, Fig. 7 presents three-dimensional configurations. The 3-D visualization shows that with increasing pressure, the prevalence of 14-coordinated clusters rises while other coordination numbers decline. This shift reflects a transition towards a more ordered, crystalline structure in the silver metallic glass.

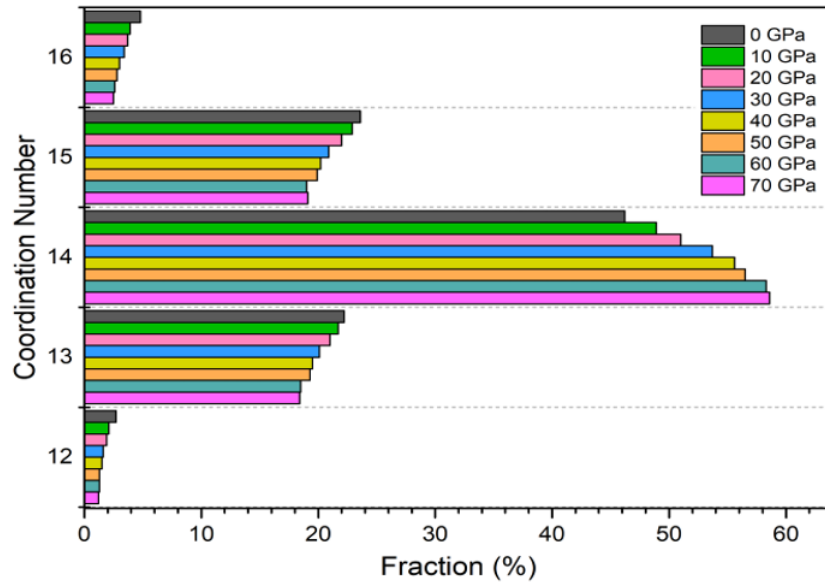


Fig. 6. The distribution of coordination number fractions in silver metallic glass at 300 K under pressures range of 0 to 70 GPa.

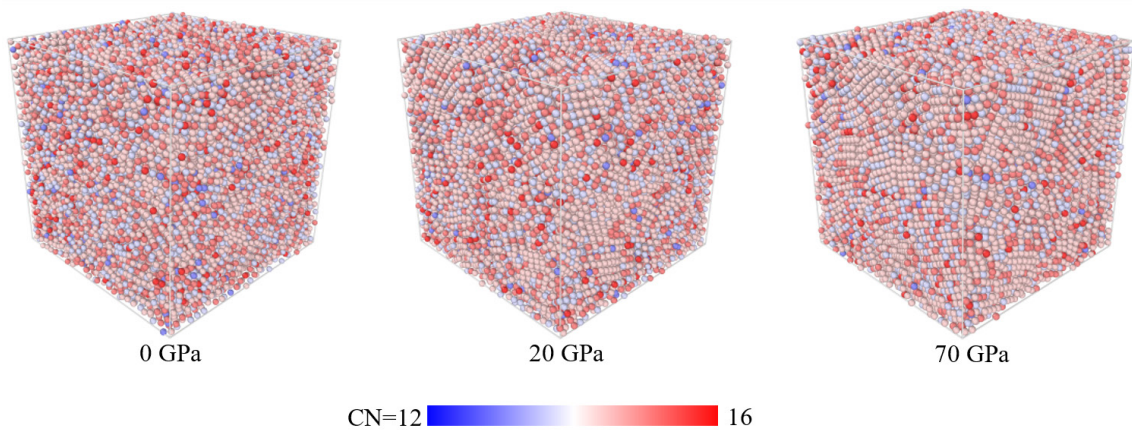


Fig. 7. 3-D visualization of coordination number distribution in silver metallic glass at ambient temperature under increasing pressures, highlighting variations in local structures and CN positions.

4. CONCLUSION

Our investigation into the behaviour of silver metallic glass under varying pressures provides significant insights into its dynamic and structural properties. The simulation results demonstrate that increased pressure leads to reduced atomic mobility, as evidenced by lower diffusion coefficients, and promotes a more ordered atomic structure, characterized by a shift towards a higher prevalence of 14-coordinated clusters. The transformation from disordered to more

crystalline structures underscores the effect of pressure on the material's internal arrangement. These findings are crucial for understanding the fundamental behaviour of metallic glasses and have implications for their practical applications, where pressure conditions may influence their performance and stability. Future research could extend these insights to other metallic glasses and explore the effects of additional variables on their structural and dynamic properties.

Author Contributions: EL HAFI Tarik: Writing – original draft, Visualization, Software, Methodology, Investigation, Data curation.

ASSOULI Soufiane: Visualization, Software, Conceptualization, Investigation.

EL KHARRAZ Abdelaziz: Software, Resources, Conceptualization, Visualization.

BAJJOU Omar: Validation, Supervision, Methodology, Conceptualization.

LACHTIOUI Youssef: Writing – review & editing, Validation, Supervision, Methodology, Investigation.

Funding: This research received no external funding.

Data Availability Statement: Data will be made available on request.

Acknowledgments: We express our gratitude for the computing assistance received from HPC-MARWAN (www.marwan.ma/hpc), made available by the National Center for Scientific and Technical Research (CNRST) in Rabat, Morocco.

Conflicts of Interest: The authors declare that they have no conflict of interest.

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