



Effect of Negative Pressure on the Structure and Diffusion Process of Silicon Dioxide at a Liquefied Nitrogen Temperature Using Molecular Dynamics Simulations

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Abstract: This study uses molecular dynamics (MD) simulations to investigate the effect of negative pressure on the structure and diffusion process of SiO_x structural units (x = 4, 5) in Silicon dioxide at a liquefied nitrogen temperature. When decreases the pressure from 0 GPa to -10 GPa at 70 K, the lengths of the links Si-Si, Si-O, and O-O initially increase and then decrease, the system size increases, and the total energy of the system increases. During the diffusion process, number of structural units SiO₄ increases, whereas the number of structural units SiO₅ decreases. The average coordination number of link Si-O is constantly 4.0, while the average coordination number of link O-O decreases from 7.0 to 6.0, leading to changes in the microstructural characteristics. This is accompanied by changes in bond angles, with SiO₄ has is 105 (degree) and SiO₅ decreasing from 90 (degree) to 85 (degree). The length of the links increases from 1.64 Å to 1.66 Å for number of structural units SiO₄ and increases from 1.68 Å to 1.74 Å for SiO₅ units. These findings provide a basis for future experimental studies aimed at the research and development of advanced materials.

Keywords: liquid nitrogen, molecular dynamics, negative pressure, number of SiO_x structural units, Silicon dioxide.

1. INTRODUCTION

Silicon dioxide (SiO₂), or silicon dioxide, is the most dominant oxide material in the Earth's crust and mantle, making it highly significant in science, technology, geophysics, and various other

fields [1-4]. Silicon dioxide exists in both liquid and crystalline amorphous forms, with its structure primarily composed of SiO₄ tetrahedra. At room temperature (300 K), the average Si/O/Si bond angle is 147 (degree), the O/Si/O bond angle is

107°, and length of the link Si-O is 1.62 Å [5-8]. The atomic-scale structure of Silicon dioxide can be investigated using various experimental and simulation methods, with Molecular Dynamics (MD) simulations being particularly favored due to their efficiency and cost-effectiveness. Recently, the scientists have employed MD simulations to examine the impact of factors such as atomic number, temperature, pressure, heating rate, and annealing time on the structure of Silicon dioxide [9], oxides like Fe₂O₃ [10-12], CaSiO₃ [13], and MgSiO₃ [14,15]. In that, the studies of Silicon dioxide structural characteristics under high temperatures and pressures, using both simulations and experimental methods, reveal a high degree of medium-range order (MRO) and strong directional bonding. These studies identify the presence of SiO₄, SiO₅, and SiO₆ units in the liquid state, with stability in the amorphous crystalline form. In Silicon dioxide glass, the SiO₄ tetrahedral structure predominates [1,16-19]. Additionally, ab-initio and first-principles MD simulation results demonstrate that the average Si/O coordination number increases from 4 to 6 as pressure rises from 0 GPa to higher [20,21]. This increase in coordination number is indicative of significant structural rearrangements under pressure, contributing to our understanding of Silicon dioxide behavior under extreme conditions. One of the key distinctions between the glassy and liquid states of Silicon dioxide is the variation in the Si/O/Si bond angle distribution. In the liquid state, this bond angle distribution becomes broader and more variable compared to the more constrained distribution in the glassy state. This variation in bond angles is a critical factor in the physical properties of Silicon dioxide, affecting everything from its viscosity to its thermal and mechanical properties. Despite these insights, certain aspects of the structural transition remain unresolved, particularly at the microscopic level. The precise nature of how local atomic arrangements evolve with changing conditions is still a subject of ongoing research. For instance, the mechanisms

driving the transition from tetrahedral to higher-coordination units under pressure are not fully understood. Studies by Karki et al. [20] and Tuan et al. [22] have further elucidated the impact of pressure and temperature on the diffusion properties of Silicon dioxide. They found that the diffusion constant can effectively reproduce the transition of Silicon dioxide from a strong to a fragile liquid state with increasing temperature and pressure. This transition is characterized by a marked change in the liquid's viscosity and flow properties, transitioning from a relatively rigid and slow-moving structure (strong liquid) to a more easily deformable and faster-moving one (fragile liquid). An unusual variation in the self-diffusion constants of both oxygen and silicon atoms is observed around 4000 K, suggesting complex underlying dynamics. This anomaly points to significant changes in the atomic mobility and interactions at high temperatures, providing new applications of Silicon dioxide in harsh conditions.

Dynamic heterogeneity (DH) in Silicon dioxide has garnered significant interest, with Vogel et al. [23] investigating it by analyzing the behavior of mobile atoms and their aggregates. They proposed that DH arises because the average size of aggregates containing freely moving atoms is larger than that of regular regions. This implies that these mobile regions exhibit enhanced dynamics compared to their surroundings, leading to heterogeneous behavior. Mizuno et al. [24] further elaborated on this by showing that neighboring mobile atoms can enhance each other's mobility, suggesting a cooperative mechanism underlying DH in Silicon dioxide liquids. This cooperative motion is believed to be the initial stage of DH, where the movement of one atom facilitates the movement of its neighbors, creating clusters of dynamically correlated atoms. Although the diffusion trajectory (DT) associated with DH has been extensively studied in supercooled Silicon dioxide liquids, some aspects remain unresolved. Specifically, gaps exist in our understanding of DH in the

liquefied gas region under negative pressure conditions [25-26]. These gaps highlight the need for further research to elucidate the behavior of Silicon dioxide under these unique conditions. Recently, the scientists have focused on the structural properties of Silicon dioxide at extremely low temperatures and varying pressures. At a temperature of 70 K and a pressure of 0 GPa [9], the structure of Silicon dioxide was examined, revealing that lengths of the links are highly stable under these conditions. For instance, length of the link Si-O in Silicon dioxide was found to be 1.64 Å [9], whereas in Mg₂SiO₄, it was slightly shorter at 1.58 Å [22]. This difference suggests that the presence of Mg²⁺ ions in the oxide compound influences length of the link Si-O, leading to a more compact structure in Mg₂SiO₄ compared to pure Silicon dioxide. Moreover, the study of Silicon dioxide within Mg₂SiO₄ under negative pressure, with pressure reduced from 0 GPa to -6 GPa, showed significant structural stability at 70 K [22]. These findings underscore the robustness of Silicon dioxide structural framework even under negative pressure, which is important for understanding its potential applications and behavior in various environmental conditions.

An intriguing question arises: how do the structural characteristics and phase transitions of SiO₄ and SiO₅ structures behave under negative pressure at the temperature of liquid nitrogen? To address this question, this study focuses on investigating the effect of negative pressure on the structure and diffusion processes of Silicon dioxide at liquid nitrogen temperature. The insights gained from this study will serve as a foundation for future

experimental research aimed at the development and manufacturing of advanced materials.

2. THE PROCEDURE FOR COMPUTATIONAL ANALYSIS

The model of Silicon dioxide consists of 1000 silicon (Si) atoms and 2000 oxygen (O) atoms, simulating a system at a liquefied nitrogen temperature of 70 K and varying negative pressures of 0, -3, -5, -7, -10 GPa, respectively. The system is condensed within a cube, the dimensions of which are determined by the formula (1) [9,22]:

$$l = \sqrt[3]{\frac{N}{\rho}} = \sqrt[3]{\frac{m_{Si}n_{Si} + m_{O}n_{O}}{\rho}} \quad (1)$$

where $m_{Si} = 26.98154$ and $m_{O} = 15.999$ are the molecular weights of silicon and oxygen, respectively. n_{Si} and n_{O} are the atomic numbers of silicon and oxygen. ρ is the chosen atomic density of 2.58 g/cm³, which closely approximates the actual density of Silicon dioxide in liquid form.

To investigate the structural characteristics using the molecular dynamics (MD) method, the entire system is immersed in the Beest-Kramer-van Santen (BKS) pair interaction force field. This force field is defined by the formula (2) with periodic boundary conditions [27]:

$$U_{ij}(r) = \frac{q_i q_j}{r_{ij}} + A_{ij} e^{-B_{ij} r_{ij}} - B_{ij} r_{ij} - C_{ij} r_{ij}^{-6} \quad (2)$$

where: r_{ij} is the distance between atoms i and j ; q_i and q_j are the charges of atoms i and j ; A_{ij} , B_{ij} and C_{ij} are potential coefficients determined by the specific characteristics of the interaction between atoms i and j , as outlined in Table 1.

Table 1. Parameters of the Silicon dioxide bulk material [9,22,27]

Silicon dioxide	Si-Si	Si-O	O-O
A_{ij} (eV)	0	18003.5773	1388.773
B_{ij} (Å ⁻¹)	0	4.87318	2.76
C_{ij} (eVÅ ⁵)	0	133.5381	175.0
$q_{i,j}$ (e)		$q_{Si} = +2.4, q_{O} = -1.2$	

This interaction potential captures the forces between atoms in the system, incorporating both short-range repulsion and long-range attraction

effects. Periodic boundary conditions are applied to the simulation cell to simulate an infinite system, allowing interactions to occur across cell

boundaries. The Verlet algorithm is utilized to integrate the equations of motion, with a time step of 0.48 fs. This algorithm accurately updates the positions and velocities of atoms at each time step, ensuring stable and efficient simulations.

To mitigate the initial configuration effect, the sample temperature was raised to 7000 K. This high temperature facilitated stable melting through a relaxation process consisting of 2×10^5 steps. Subsequently, the sample temperature was gradually reduced back to 70 K over 2×10^5 steps. Next, an isothermal-isobaric (NPT) ensemble was applied to stabilize the model at 70 K and a pressure of 0 GPa, encompassing approximately 2×10^5 steps. This stabilized sample, referred to as the 0 GPa sample, served as the basis for subsequent analyses. To explore the effects of pressure, five additional samples were generated at 70 K with pressures of 0, -3, -5, -7, and -10 GPa. These samples underwent relaxation through model adjustment procedures. Each sample was subjected to equilibrium simulations in the canonical (NVE) group, involving 2×10^5 steps to achieve equilibrium. Additional simulation runs spanning 5×10^5 steps were conducted to capture detailed structural and dynamic data.

To investigate the impact of negative pressure on the structural characteristics of Silicon dioxide, a limiting radial distance cut-off ($r_{\text{cut-off}}$) of 2.28 Å is defined. This cut-off distance is chosen to coincide with the position of the first peak of the pair radial distribution function (RDF), denoted as $g_{\text{Si-O}}(r)$, as determined by the formula (3) [9,22]:

$$g(r) = \frac{V}{N^2} \left\langle \frac{\sum_i n_i(r)}{4\pi r^2 \Delta r} \right\rangle \quad (3)$$

where: r , $n_i(r)$, V , N , $g(r)$ denote respectively, length of the links, coordinates, volume, and the pair radial distribution function (RDF).

Subsequently, the average coordination number is calculated using formula (4) [9,22]:

$$\text{CN} = 4\pi\rho \int_0^{r_1} g(r) r^2 dr, \quad (4)$$

where r_1 is the first peak position of RDF.

The bond angle is determined by the following formula (5) [9,22]:

$$\cos \alpha = \frac{2r_{\text{Si-O}}^2 - r_{\text{Si-Si}}^2}{2r_{\text{Si-O}}^2}, \quad (5)$$

where: α = Si-O-Si

Additionally, the counts of SiO_4 and SiO_5 structural units are obtained by employing the coordination number circle. The entire heating process of Silicon dioxide is executed using the Nosé-Hoover equation [28,29].

3. RESULTS AND DISCUSSION

3.1. Effect of negative pressure on the structure of Silicon dioxide

To investigate the structural morphology of Silicon dioxide, modeling methods were employed for observation, and the findings are depicted in Figure 1.

Upon examining the findings presented in Figure 1, it becomes evident that Silicon dioxide manifests as an oxide material comprising two Si atoms and oxygen atoms arranged within a cube structure, influenced by the BKS interaction force field and subject to periodic boundary conditions. With a configuration of 1000 Si atoms and 2000 O atoms, Si and O atoms are visually represented in red and blue, respectively, exhibiting a relatively uniform distribution. This observation pertains to the state of Silicon dioxide at liquefied nitrogen gas temperature, approximately corresponding to 70K, under a pressure of 0 GPa (Figure 1a). As the pressure (P) is gradually reduced from $P = 0$ GPa to $P = -3$ GPa (Figure 1b), -5 GPa (Figure 1c), -7 GPa (Figure 1d), and -10 GPa (Figure 1e), notable alterations occur in the volume (depending of size l) of Silicon dioxide. The volume expands incrementally from $l = 3.44$ nm at 0 GPa to $l = 3.50$ nm, 3.55 nm, 3.60 nm, and 3.68 nm, respectively, as the pressure decreases. Simultaneously, there is an increase in the total energy of the system (E_{tot}) from $E_{\text{tot}} = -53408$ eV at 0 GPa to $E_{\text{tot}} = -53389$ eV, -53345 eV, -53284 eV, and -53112 eV, respectively.

This phenomenon can be attributed to the reduction in pressure causing an expansion of the Silicon dioxide volume and a subsequent decrease in atom density within the Silicon dioxide matrix, resulting in an overall increase in the system's total energy. This rise in energy within the temperature range of liquefied nitrogen gas presents new avenues for research in Silicon dioxide, offering insights that could shape future advancements in materials applications.

To answer this question, we examine the relationship between pressure (P), size (l), and the total energy of the system (E_{tot}) by studying Figure 2.

The findings reveal a first-order function between pressure (P) and size (l), demonstrating a linearly proportional relationship (Figure 2a). Conversely, the relationship between P and the total energy of the system (E_{tot}) manifests as a second-order linear correlation, presenting a proportional curve. As pressure decreases, both the size and total energy of the system increase. Subsequently, the microstructural attributes of Silicon dioxide are elucidated through the radial distribution function (RDF), computed via formula (3), with the outcomes depicted in Figure 3.

The obtained results illustrate the RDF outcomes, which are characterized by the lengths of the links Si-Si, Si-O, and O-O. Upon decreasing the pressure from 0 GPa to -10 GPa, several notable changes occur. Specifically, the length of the links Si-Si change about from 3.20 Å to 3.33 Å, while the RDF height of the links Si-Si change about from 4.65 to 6.60 (Figure 3a). Similarly, the length of the links Si-O change about from 1.64 Å to 1.66 Å, accompanied by changes in the RDF height of the links Si-O change about from 39.94 to 45.93 (Figure 3b). Additionally, the length of the links O-O increases from 2.62 Å to 2.66 Å, while the RDF height of the links O-O changes from 5.19 to 4.79 (Figure 3c). Notably, the radial distribution function exhibits a circular peak at the second peak of the RDFs, indicating the crystalline amorphous

state of Silicon dioxide, with the largest length of the link between Si and O evidenced by the peak's sharpness. To ensure the accuracy of the Silicon dioxide results obtained, a comparison is conducted with previously obtained results, as detailed in Table 2.

The results obtained from Table 2 reveal a good correlation between the lengths of the links Si-Si, Si-O, and O-O as determined by RDF analysis and the corresponding data for Silicon dioxide under two distinct sets of conditions. Firstly, when Silicon dioxide is subjected to the temperature of liquefied nitrogen (N_2) at 70 K and a pressure of 0 GPa [9], secondly, at an extreme temperature of 3200 K and a pressure of 0 GPa [1, 2, 5, 20, 28, 29] and it used in applications at negative pressure [30]. This comparison underscores a remarkable similarity between the length of the links observed in Silicon dioxide under cryogenic conditions and those at a significantly higher temperature, indicative of an amorphous structure akin to Silicon dioxide at 3200 K. Additionally, it is important to study the average coordination number of the links. The results of this analysis are illustrated in Figure 4. This examination of the average coordination number provides crucial insights into the structural arrangement and bonding patterns of the material, complementing the assessment lengths of the links conducted through RDF analysis.

The results indicate that the average coordination number (CN) for the link Si-Si is 4 (Figure 4a), while for Si-O, it remains at 4 (Figure 4b). In that, the average coordination number of the links O-O decreased from 6.0 to 5.0 (Figures 4b and 4c). Interestingly, when the pressure decreases, there's no change in the average coordination numbers of links Si-Si and Si-O in terms of atomic number. However, there's a significant alteration observed in the link O-O. This observation suggests that as pressure decreases, the size of Silicon dioxide increases, resulting in an increase in the length of the link O-O.

Consequently, the total energy of the system increases, leading to an increase in the number of atoms bonded via the links O-O in Silicon dioxide. This change in the system prompts a consideration of whether it influences the number of structural units and the angular distribution. These potential ramifications will be discussed in detail in the subsequent section.

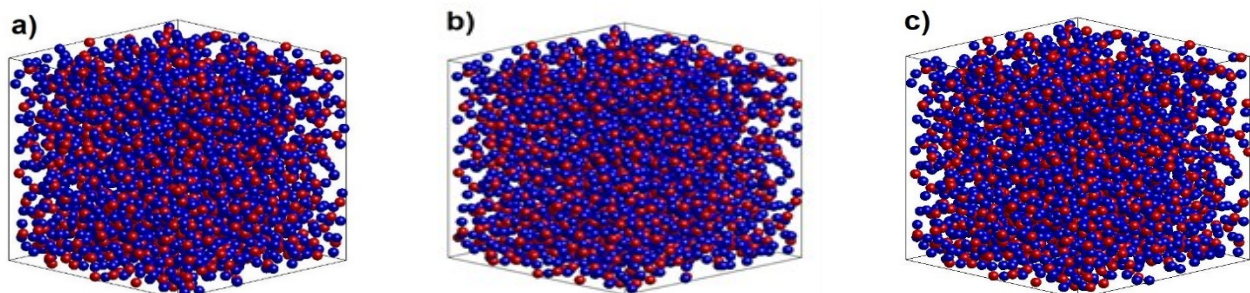
3.2. Effect of negative pressure on the diffusion process of Silicon dioxide

In the context of negative pressure at a liquefied nitrogen temperature, Figure 5 illustrates the representation of structural units SiO_4 and SiO_5 . This depiction provides valuable insights into the composition and arrangement of these structural units within the Silicon dioxide material under such conditions.

The findings reveal important insights into the behavior of SiO_4 and SiO_5 structural units under the conditions of a liquefied nitrogen temperature and varying pressure. At a pressure of 0 GPa, the SiO_4 structure comprises 1723 atoms, featuring a consistent Si-O-Si bond angle of 105 (degree). Similarly, there are 36 SiO_5 atoms, showcasing a Si-O-Si bond angle of 90 (degree). Remarkably, as the pressure is reduced from 0 GPa to -3, -5, -7, and -10 GPa, certain intriguing dynamics unfold. The SiO_4 bond angle remains steadfast at its 105 (degree) (Figure 5a), whereas the SiO_5 bond angle gradually diminishes from 90 (degree) to 85 (degree) (Figure 5b). This shift in bond angles coincides with a reduction in the number of SiO_4 and SiO_5 atoms. Specifically, the count declines from 1723 to 1709, 1650, 1588, and 1455 atoms for SiO_4 , and from 36 to 20, 19, 15, and 5 atoms for SiO_5 , respectively, as pressure decreases. These

observations align seamlessly with earlier findings indicating that as pressure decreases, lengths of links Si-Si and Si-O remain unaltered, while length of the link O-O increases. Moreover, to augment these results, an investigation into angular distance distribution was conducted, the outcomes of which are depicted in Figure 6.

The results elucidate the angular distance distribution of SiO_4 and SiO_5 structural units at 0 GPa pressure, unveiling intriguing patterns. At this pressure, SiO_4 exhibits a distribution of 1.64 Å with 1319 atoms, while SiO_5 showcases a distribution of 1.68 Å with 14 atoms. As the pressure decreases from 0 GPa to -10 GPa, notable transformations emerge. The distance distribution expands from 1.64 Å to 1.66 Å for SiO_4 , accompanied by changes in atom count from 1319 to 1443, 1326, 1203, and 1052 (Figure 6a). Similarly, for SiO_5 , the distribution increases from 1.68 Å to 1.7, 1.72, and 1.74 Å, while the atom count dwindles from 14 to 6, 5, 3, and 2 (Figure 6b). These findings signify that decreasing pressure from 0 GPa to -10 GPa at liquefied gas temperatures engenders an enlargement in Silicon dioxide dimensions. Consequently, the system's total energy increases, leading to a reduction in atom density and an elongation lengths of the links Si-Si, Si-O, and O-O. Notably, while the average coordination numbers of links Si-Si and Si-O remain unaltered, the average coordination number of the link O-O undergoes significant variation. Moreover, the distance distribution of structural units experiences augmentation. These compelling outcomes lay a robust foundation for future experimental endeavors aimed at researching and manufacturing advanced materials.



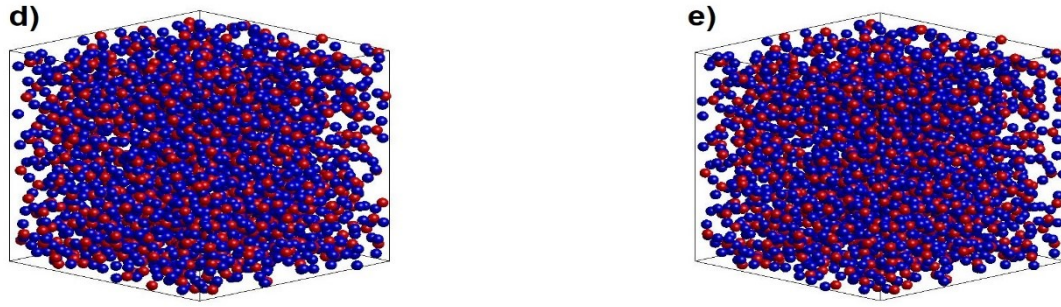


Figure 1. Shape of Silicon dioxide at N₂ liquefied gas temperature under various negative pressures as: 0 GPa (a), -3GPa (b), -5GPa (c), -7GPa (d), -10GPa (e)

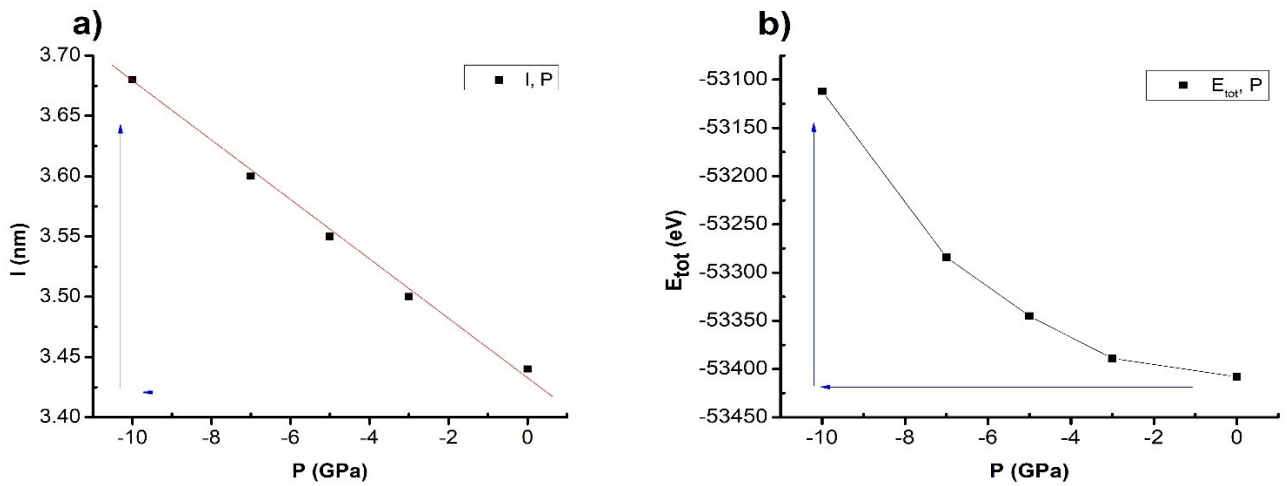


Figure 2. (a) Relationship between pressure and size, and (b) total energy of the system

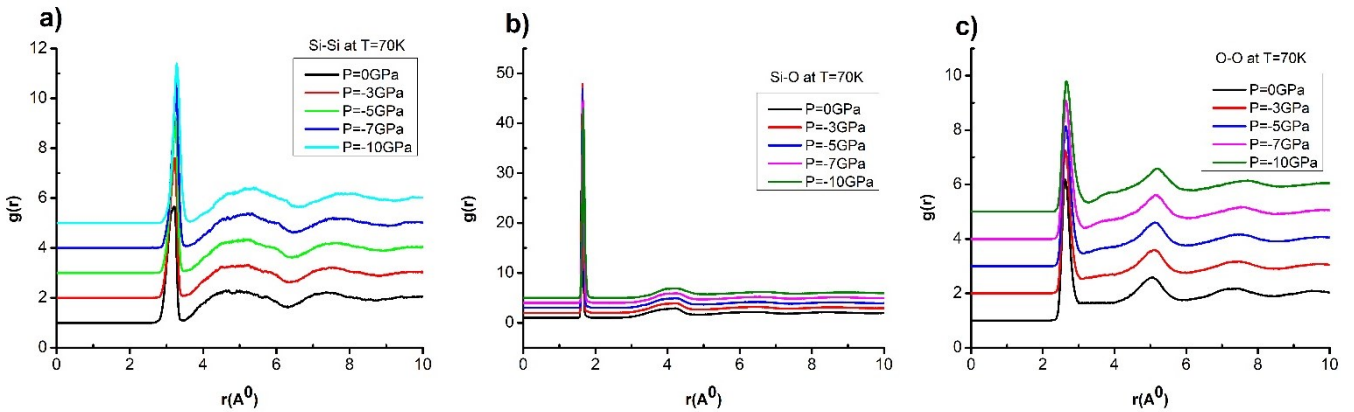


Figure 3. (a) Radial distribution function of the links Si-Si, (b) Si-O, (c) O-O of Silicon dioxide at N₂ liquefied gas temperature under various negative pressures

Table 2. A comparative analysis between the obtained results and those from previous studies

Si-Si (Å)	Si-O (Å)	O-O (Å)
4.65	1.64	2.62
3.58 [20]	1.63 [20]	2.63 [20]
-	1.60 [28]	-
-	1.63 [1]	-
3.08 [2]	1.62 [2]	2.60 [2]
3.08 [5]	1.61 [5]	2.63 [5]
3.12 [29]	1.62 [29]	2.65 [29]
3.20 [9]	1.64 [9]	2.64 [9]

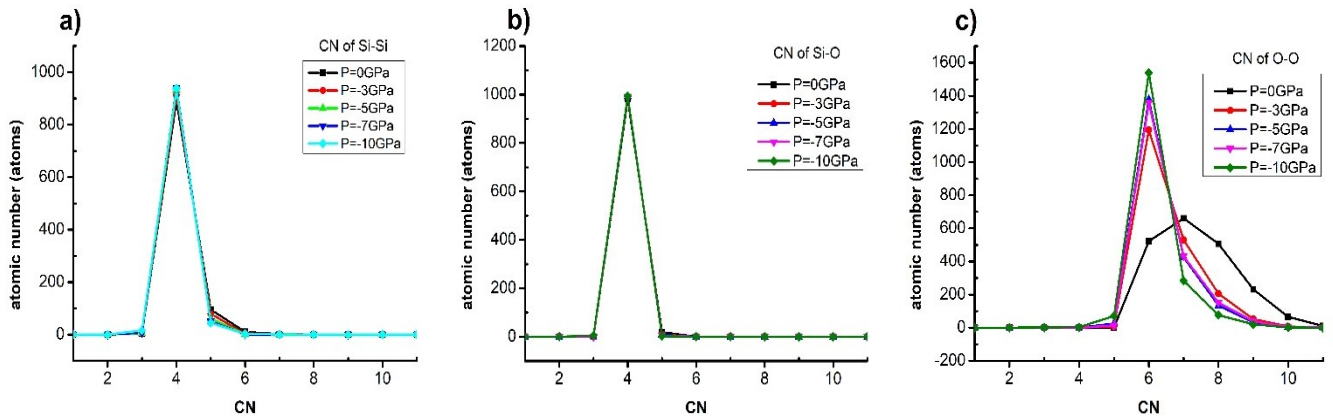


Figure 4. Average coordination number of the links Si-Si (a), Si-O (b), O-O (c) of Silicon dioxide at N₂ liquefied gas temperature under various negative pressures

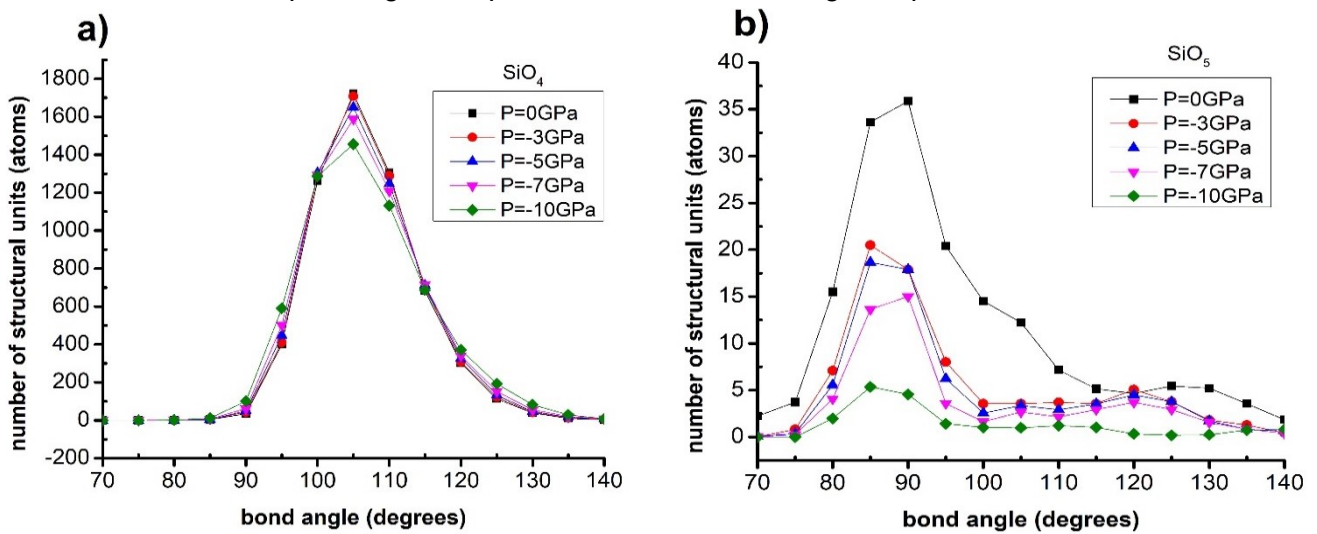


Figure 5. Number of structural units of SiO₄ (a), SiO₅ (b) at N₂ liquefied gas temperature under various negative pressures

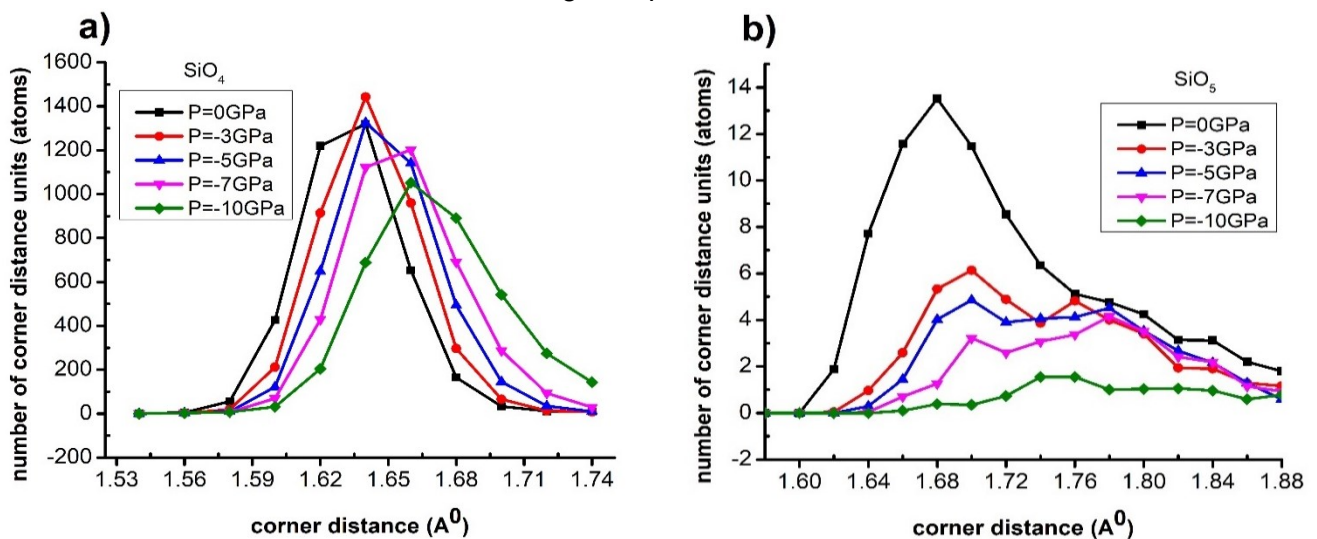


Figure 6. Angular distance distribution of SiO₄ (a), SiO₅ (b) at a liquefied nitrogen temperature under various negative pressures

4. CONCLUSIONS

The investigation into the impact of negative

pressure on the microstructural characteristics and diffusion process of Silicon dioxide at a liquefied

nitrogen temperature of 70 K employing the molecular dynamics method has yielded insightful revelations. As the pressure diminishes from 0 GPa to -10 GPa under these conditions, the lengths of the links Si-Si, Si-O, and O-O undergo a notable pattern of increase followed by decrease. Specifically, length of the links Si-Si increases from 3.20 Å to 3.33 Å, subsequently decreasing to 3.28 Å. Similarly, length of the links Si-O increases from 1.64 Å to 1.66 Å, while length of the links O-O increases from 2.62 Å to 2.66 Å. Consequently, the size of Silicon dioxide increases from 3.44 nm to 3.68 nm, accompanied by an increase in the total energy of the system from -53408 eV to -53112 eV. Despite these fluctuations, the average coordination numbers of links Si-Si and Si-O remain constant at 4.0, while that of O-O declines from 7.0 to 6.0. This alteration results in a significant change in the structural units number of SiO₄, SiO₅, with the density of SiO₄ atoms increasing and SiO₅ decreasing. Notably, the bond angle remains at 105 (degree) for SiO₄ but decreases from 90 (degree) to 85 (degree) for SiO₅. Additionally, the angular distance distribution exhibits an increase from 1.64 Å to 1.66 Å for SiO₄ and from 1.68 Å to 1.74 Å for SiO₅. These findings hold considerable promise for future experimental endeavors aimed at advancing materials manufacturing processes.

Author Contributions:

Ş.Ț.: writing original draft preparation and reviewing. T.T.Q., U.S., B.M. K.: writing original draft preparation. D.N.T.: writing original draft preparation, conceptualization, software, investigation, resources, formal analysis, data curation, project administration, funding acquisition, visualization, methodology, and supervision. All authors have read and agreed to the published version of the manuscript.

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