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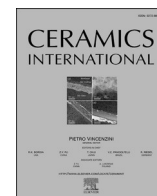
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Machine learning–assisted structural characterization of ring size distribution in Sr-doped bioactive glasses: A molecular dynamics study

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ABSTRACT

Bioactive glasses (BGs) are promising biomaterials in tissue engineering, orthopedics, and dentistry due to their ability to bond with living tissue. In this study, the atomic structure of strontium-substituted melt-quenched 60SiO₂–(40–x)CaO–xSrO BGs (x = 0–20 mol%) was investigated using molecular dynamics (MD) simulations in LAMMPS. Structural data from radial distribution functions (RDFs) were used to train a two-dimensional convolutional neural network (2D CNN), which predicted ring size distribution (RSD) based on 10×100 matrices of atomic pair distributions. Short-range structural analysis showed a consistent Si–O bond length (1.607 Å) across samples, while Sr–O bond length was 2.57 Å with coordination numbers decreasing from 7.25 to 6.89. The Si–O–Si angle widened from 148.97° to 149.65° with rising Sr content, reflecting network expansion. Network-level parameters such as Qⁿ unit distribution, bridging/non-bridging/free oxygens, and network connectivity (NC) were also evaluated. NC slightly decreased from 2.687 to 2.675, with minimal BO/NBO changes, and overall density rose due to the higher molar mass of Sr. Taken together, the study showed the effective integration of MD and machine learning framework, and the CNN accurately predicted RSD, achieving low MSE and high coefficient of determination R².

1. Introduction

Bioactive glasses (BGs) are considered to be one of the most innovative biomaterials in dental applications, orthopedics, and tissue engineering (TE) [1–3]. With a unique combination of biological, chemical and physical properties, these biomaterials have the ability to form direct bonds with living tissues and have been widely used in stimulating desirable biological responses for bone and dental repair [4–6]. Since the invention of 45S5 BG by Hench in the 1970s, significant advances have been made in the composition, structure and performance of BGs [7,8]. Although 45S5 is known as the mainstay in the development of BGs, limitations such as too rapid dissolution in vivo and high tendency to crystallization/poor sinterability upon thermal treatment have led researchers to move towards more optimal compositions [9]. In this regard, simpler binary systems such as SiO₂–CaO without the presence of sodium have been considered [10–12]. The 60SiO₂–40CaO composition has been proposed as one of the most stable and tunable compositions in terms of structure and biological performance, which has features such as higher thermal stability, more uniform structure,

and the ability to finely control the ion release behaviors upon doping with small amounts of therapeutic metallic elements [13].

Strontium (Sr) is one of the key elements in bone biology that has attracted much attention in the field of BG design in recent years [14–18]. The presence of Sr²⁺ in the biological environment has positive effects on bone regeneration [19,20], including stimulating osteoblast differentiation [21], inhibiting osteoclast activity [22], and increasing bone mineral density [23]. Various experimental studies have shown that adding strontium to the composition of BGs not only improves ion release and faster formation of the hydroxyapatite layer, but also improves mechanical properties and biostability [24,25]. However, the exact role of Sr in the BGs network structure and its effects on the arrangement of the interlayer structure, such as the ring size distribution, are still not fully understood.

The structure of silicate-based BGs has been studied at both short-range and medium-range levels [26]. At the short-range level, parameters such as bond length and coordination number (CN) have been considered, while at the medium-range level features such as tetrahedral angle distribution, ring size distribution (RSD), and connectivity

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between structural units have been crucial in previous researches [27–32]. As an indicator of how SiO₄ tetrahedra are connected in a three-dimensional network, RSD provides a deep understanding of the network density, ion accessibility, and transport pathways [33–37]. In other words, any change in the BG composition, such as replacing Ca²⁺ with Sr²⁺, can lead to changes in the arrangement of these rings, ultimately affecting macroscale properties such as bioactivity and dissolution rate [38].

Over the last few years, molecular dynamics (MD) simulations have been used as a powerful tool for modeling and analyzing the structure of amorphous BGs [39–42]. By providing accurate atomic data, these simulations allow extracting information such as the Radial Distribution Function (RDF) [43], bond angles [44], ring structures [45], and ion interactions [46]. However, the outputs from MD usually contain a large volume of complex data without clear structure, and their analysis requires time, expertise, and high computational resources, especially for extracting high-level features such as RSD. In such a context, machine learning (ML) is considered as a very valuable complementary tool for analyzing complex data and extracting hidden patterns from them [47, 48]. In the field of BGs, ML applications are just beginning to develop and can be used to predict properties such as ion release behavior [49], bioactivity [50], ring distribution [39], and mechanical properties [51]. One of the effective ML architectures for spatial data analysis is 2D convolutional neural networks (CNNs) [52]. These networks are particularly well-suited for analyzing tensorial data such as images or 2D RDF maps, as they are able to extract spatial features and local relationships in a hierarchical manner.

In this study, for scientific investigation of the effect of SrO substitution on the melt-derived BG structure, first, the RDF composite transformed into a 2D map was used as the CNN input so that the neural network model could predict the RSD for Sr-doped BGs with a base composition of 60SiO₂-40CaO. BGs with different percentages of SrO (0, 1, 3, 5, 8, 10, 15, and 20 mol%) were simulated using large-scale atomic/molecular massively parallel simulator (LAMMPS) software. Second, the output of structural data such as RDF and RSD were used to prepare a set of training data. The RDFs were transformed into 2D maps and fed to the CNN so that the model could automatically predict the RSD. In addition to the scientific investigation of the effect of Sr on the network structure, this framework was also introduced as a generalizable deep learning model. Specifically, short-range structure, medium-range structure, and the results of the CNN model are investigated. Finally, the viability of this approach to predict the RSD results was evaluated, and an optimal Sr-doped BG composition was selected based on the RSD results.

2. Methodology

2.1. Simulation details

All BG compositions shown in Table 1 had a set of partial charge pairwise potentials. For every BG simulation, the potentials' short-range interaction has the Buckingham form, while the potentials' long-range

interaction has the Coulomb form. Buckingham potentials forms are described by Eq. (1), where A, ρ and C are Buckingham potentials parameters and r is the distance between two atoms.

$$V(r) = A \exp\left(-\frac{r}{\rho}\right) - \frac{C}{r^6} \quad \text{Equation (1)}$$

Buckingham potentials shown in Table 2 are used as in the study by Du et al. for Si-O, Ca-O, Sr-O and O-O pairs parameters [53].

To start the simulation process, atoms were arranged at random positions within the simulation box to produce an amorphous structure [54]. Moreover, the initial density for BGs was set similar to experimental densities. To simulate the synthesis of the BGs, the LAMMPS package was utilized as a tool to replicate the melt-quenching process [55]. Additionally, the equation of motion was integrated using the velocity Verlet algorithm with a time step of 1 fs, and the long-range Coulomb interactions were computed using the Ewald sum method [56]. First, the simulation box was run for 5 ps in the NVE ensemble as a relaxation step. Then, the system was heated to 5000 K over 20 ps and maintained at this temperature for 150 ps in the NVT ensemble to ensure complete melting and homogenization of the structure, as well as to eliminate the effects arising from the random initial placement of atoms. Subsequently, the system was cooled to 3000 K at a cooling rate of 1 K/ps under the NVT ensemble. At 3000 K, the NPT ensemble was employed to obtain the equilibrium density of the structure, where both temperature and pressure were controlled and the simulation box volume was allowed to vary until equilibrium was reached. For this purpose, the system was maintained at 3000 K and 1 atm for 100 ps to achieve the equilibrium density. In the next stage, the simulation box was cooled from 3000 K to 300 K at a cooling rate of 1 K/ps under the NPT ensemble. Finally, the system was run for 100 ps under the NPT ensemble and for another 100 ps under the NVT ensemble to ensure that the temperature, density, and energy of the structure had reached equilibrium. Ultimately, for structural analyses, the system was simulated for 20 ps under the NVE ensemble.

2.2. Statistical analysis

Three sets of simulations were performed to acquire precise and statistically significant differences, and the results were given as means $\pm$ standard deviation (SD). GraphPad Prism software (version 10.3.1) was utilized to statistically analyze the results.

2.3. Machine learning approach

In this study, CNN was employed to predict the RSD in Sr-doped BGs. The approach consists of three primary components: the calculation of RSD, the transformation of 3D atomic positions into a 2D matrix using the RDF, and the application of a 2D CNN for prediction.

2.3.1. Ring size distribution calculation

The RSD was calculated using the algorithm proposed by Yuan et al. [57]. This algorithm identifies rings within the atomic structure by finding the shortest paths between atoms using Dijkstra algorithm, constrained by a specified cutoff distance. To implement this algorithm, an expanded dataset was processed for periodicity, and the set of corner Si atoms were chosen as reference nodes. Fig. 1 represents the flowchart of the RSD algorithm. The algorithm, based on Yuan and Cormack [57],

Table 1
Simulation details for different BGs compositions.

BGs	Number of Si atoms	Number of Ca atoms	Number of O atoms	Number of Sr atoms	Total number of atoms
Sr0	3000	2000	8000	-	13000
Sr1	3000	1950	8000	50	13000
Sr3	3000	1850	8000	150	13000
Sr5	3000	1750	8000	250	13000
Sr8	3000	1600	8000	400	13000
Sr10	3000	1500	8000	500	13000
Sr15	3000	1250	8000	750	13000
Sr20	3000	1000	8000	1000	13000

Table 2
Buckingham potential parameters for Si-O, Ca-O, P-O, and O-O bonds.

Pairs	A (eV)	ρ (Å)	C (eV/Å ⁶)
Si ^{+2.4} -O ^{-1.2}	13702.905	0.193817	54.681
Ca ^{+1.2} -O ^{-1.2}	7747.1834	0.252623	93.109
Sr ^{+1.2} -O ^{-1.2}	14566.637	0.245015	81.773
O ^{-1.2} -O ^{-1.2}	2029.2204	0.343645	192.58

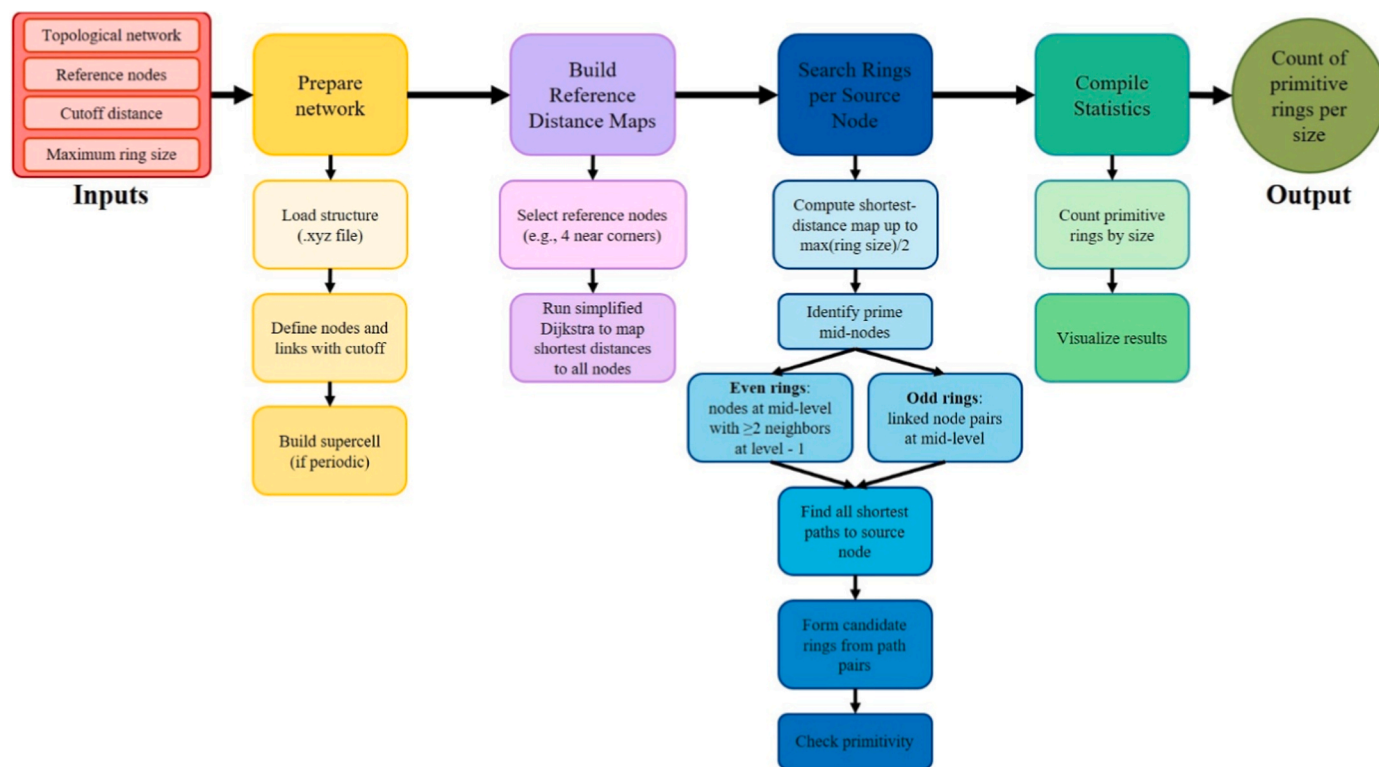


Fig. 1. Flowchart of the RSD algorithm.

efficiently calculates primitive ring statistics in topological networks, such as Sr-doped BGs, by identifying rings that cannot be decomposed into smaller ones. The code here is a modification of a previously-developed one in Julia by Morrow [58]. It started by preparing the network, loading atomic structure data, defining nodes and links using a cutoff distance (e.g., 2.0 Å for Si-O bonds), and building a supercell for periodic systems. Four reference nodes were selected to compute shortest-distance maps to all nodes using a simplified Dijkstra algorithm, avoiding large matrices. For each source node (e.g., silicon atom), a shortest-distance map was generated up to the maximum ring size (e.g., 25). Prime-mid-nodes were identified: for even rings, nodes with at least two neighbors one level closer; for odd rings, linked node pairs at the mid-level. All shortest paths from prime-mid-nodes to the source were found, forming candidate rings. The primitivity of each ring was verified by checking for shorter paths between check-nodes and mid-nodes using reference maps. Primitive rings were counted by size and output for analysis. This approach reduced memory usage and enabled efficient large-ring analysis.

2.3.2. Radial distribution function (RDF) transformation

To convert the 3D positions into a 2D matrix suitable for CNN input, RDF was utilized. The RDF quantified the probability of finding an atom at a given distance from a reference atom, offering a statistical representation of the material's atomic structure. The RDF was computed for ten specific atom pairs: Si-Si, Si-O, Si-Ca, Si-Sr, O-O, O-Ca, O-Sr, Ca-Ca, Ca-Sr, and Sr-Sr. The calculation used 0.05 Å bin size, determining the resolution of distance bins, and 5 Å as maximum radius, setting the upper limit of the radial range. For each dataset, the RDF feature vector formed a 10×100 matrix, where each row corresponds to one of the ten atom pairs, and each column represents a distance bin. This matrix served as the input to the CNN model.

2.3.3. 2D convolutional neural network

A 2D CNN was developed to predict the RSD from the RDF features. The dataset comprised eight samples, with seven used for training and

one reserved for testing. The CNN architecture was designed as depicted in Fig. 2.

The network takes a 2D input of size $[N_{\text{pairs}} \times 100 \times 1]$. This is followed by two convolutional blocks. The first block consists of a 2D Convolutional layer (3×3 filter, 16 channels, 'same' padding), followed by Batch Normalization and a ReLU activation. The second block uses a 2D Convolutional layer (3×3 filter, 32 channels, 'same' padding), Batch Normalization, a ReLU activation, and a 2×2 Max Pooling layer with a stride of 2. Finally, a Fully Connected layer maps the extracted features to the 12 output targets, followed by a regression layer. The network was trained using the Adam optimizer with a learning rate of 10^{-3} , a maximum of 500 epochs, and a full-batch approach where the mini-batch size is equal to the number of training samples. Furthermore, rather than relying on standard dropout, a rigorous k-fold (leave-one-out) cross-validation strategy was employed. The performance of the CNN model was assessed using the single test dataset, which was excluded from the training process. Three evaluation metrics were calculated: Mean Squared Error (MSE), Coefficient of Determination (R^2), and Pearson's Correlation Coefficient.

3. Results and discussion

3.1. Short-range structure

Fig. 3 shows the RDF for Si-O, Ca-O, Sr-O and O-O bonds. Accordingly, the distribution of Si-O bond lengths at different distances can be observed. The average Si-O bond length was calculated from 0.0 Å to 2.0 Å and the calculated values is shown in Table 3. For all the simulated BGs, the average Si-O bond length was 1.607 Å, which is consistent with previous literature. According to the results reported by Abd El-Moneim [59], the Si-O bond length was estimated to be 1.61 Å, which is the same value also computed by Marchin et al. [60]. Moreover, in the study of Taniguchi et al. [61], the Si-O bond length was obtained to be 1.62 Å. Fig. 3 presents the Ca-O RDF, in which a peak was observed in the range of 2.38 Å, indicating that most of the Ca-O bonds had a bond length of

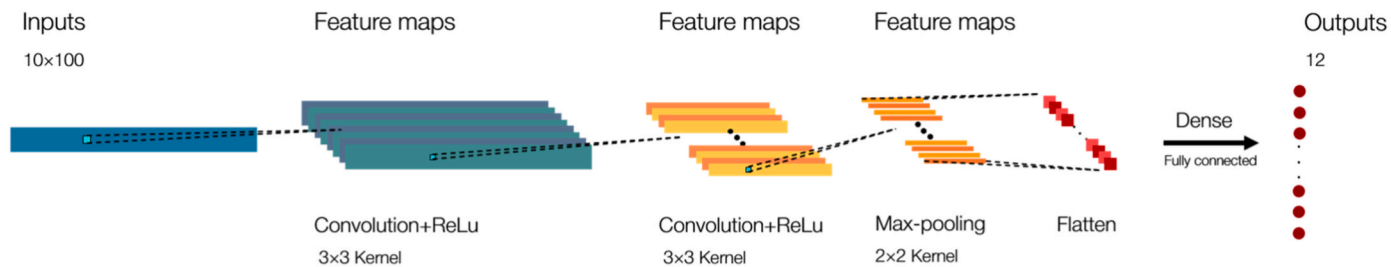


Fig. 2. CNN network architecture.

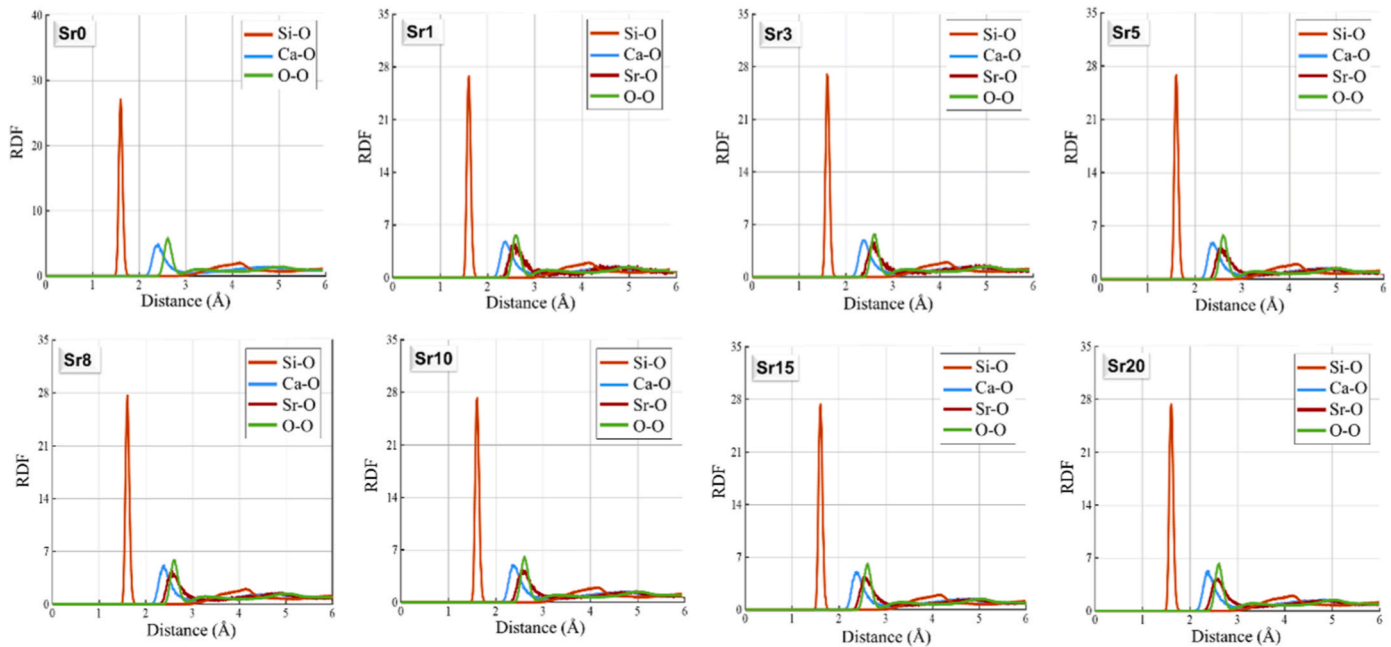


Fig. 3. RDF curves of the Sr-doped BGs for Si-O, Ca-O, Sr-O, and O-O bonds.

Table 3
Bond length, bond angle, and Coordination numbers in simulated BGs.

BGs	Si-O (Å)	Si-O (CN)	Sr-O (Å)	Sr-O (CN)	Ca-O (Å)	Ca-O (CN)	O-Si-O (°)	Si-O-Si (°)	O-O (Å)
Sr0	1.607 ± 0.015	4 ± 0.024	-	-	2.39 ± 0.013	6.22 ± 0.057	109.35 ± 0.040	148.97 ± 0.58	2.61 ± 0.021
Sr1	1.607 ± 0.020	4 ± 0.026	2.56 ± 0.019	7.25 ± 0.061	2.39 ± 0.019	6.23 ± 0.043	109.36 ± 0.043	149.16 ± 0.49	2.60 ± 0.022
Sr3	1.607 ± 0.012	4 ± 0.019	2.57 ± 0.031	7.05 ± 0.034	2.38 ± 0.020	6.18 ± 0.074	109.36 ± 0.051	149.28 ± 0.52	2.61 ± 0.018
Sr5	1.607 ± 0.015	4 ± 0.013	2.56 ± 0.035	7.05 ± 0.015	2.37 ± 0.016	6.23 ± 0.080	109.36 ± 0.048	149.31 ± 0.61	2.60 ± 0.015
Sr8	1.608 ± 0.019	4 ± 0.010	2.57 ± 0.028	7.00 ± 0.063	2.37 ± 0.015	6.16 ± 0.056	109.36 ± 0.053	149.10 ± 0.55	2.61 ± 0.025
Sr10	1.608 ± 0.023	4 ± 0.021	2.57 ± 0.015	6.96 ± 0.074	2.37 ± 0.026	6.15 ± 0.064	109.36 ± 0.052	149.53 ± 0.50	2.61 ± 0.026
Sr15	1.608 ± 0.014	4 ± 0.018	2.57 ± 0.021	6.92 ± 0.029	2.39 ± 0.029	6.11 ± 0.053	109.36 ± 0.043	149.31 ± 0.68	2.62 ± 0.018
Sr20	1.608 ± 0.017	4 ± 0.020	2.60 ± 0.016	6.89 ± 0.093	2.37 ± 0.018	6.11 ± 0.081	109.35 ± 0.052	149.65 ± 0.61	2.62 ± 0.019

2.38 Å. Meanwhile, the Sr-O curve in Fig. 3 shows that the peaks were located around 2.6 Å. Unlike the Ca-O bond, the Sr-O bond exhibited a longer bond length, which could be attributed to the larger atomic radius of the Sr atom [62]. In the study of Martin et al. [63], the length of Ca-O bonds was reported to be 2.33 Å, while in a report by Jamieson et al. [64], the length of Ca-O bonds was reported to be in the range of 2.3 Å to 2.4 Å. In another study by Pedone et al. [65] the of Ca-O bond length was 2.30 Å, and Honda et al. [66] reported the length of Sr-O bonds to be approximately 2.59 Å, which was in good agreement with the results of this study. The O-O curve in Fig. 3 also shows that the oxygens in the structure were mainly located at a distance of approximately 2.6 Å from each other, which can be concluded by averaging the distance from 0.0 to the first valley in the O-O curve. The results reported in the study of Marchin et al. were in line with the results of this

study for BGs containing a high amount of SiO₂ [60]. Additionally, in the study of Du et al. [67], the values of the O-O bond length were equal to 2.62 Å, and in the study of Rao [68], this value was approximately equal to 2.6 Å.

By integrating the RDF and using Eq. 2, the X-O CN (X: Si, Ca & Sr) can be obtained and the results are presented in Fig. 4. It is concluded that the average Si-O CN in all the BGs was equal to 4. It should be noted that a cutoff radius of 2.0 Å was used to calculate the Si-O CN regarding the first coordination shell. These results indicated that the network units were tetrahedral, and were in good agreement with other researches [60,69,70]. As shown in Fig. 4 the Ca-O CN changed with increasing the distance even after a distance of 2.38 Å. In this study, a cutoff radius of 3.1 Å was considered for the first coordination shell of Ca-O and the CN was reported to be between 6.1 and 6.2. According to

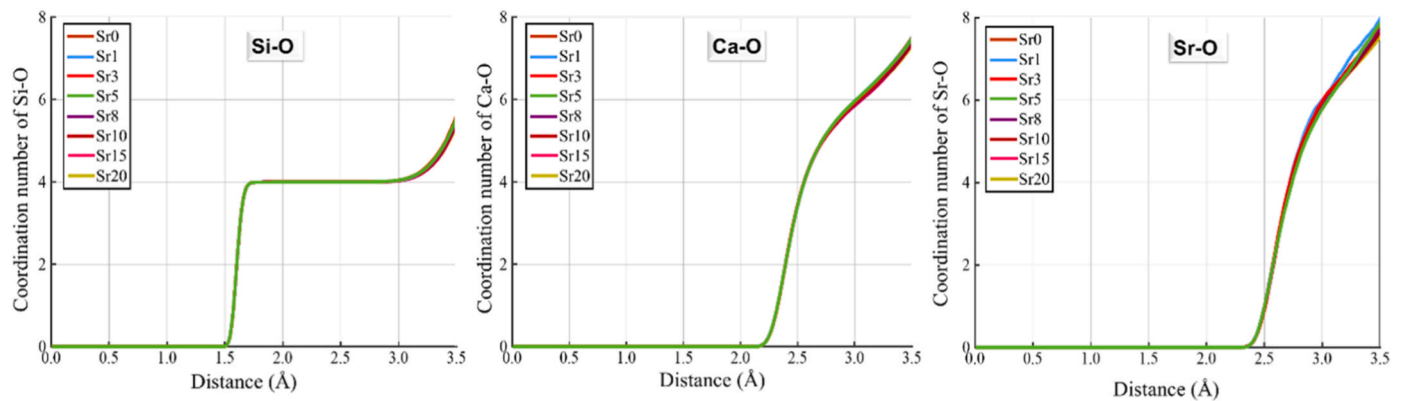


Fig. 4. CN calculations of Sr-doped BGs for Si-O, Ca-O, and Sr-O bonds.

the study of Pedone et al. [65], the average Ca-O CN was in good agreement with the results of this study, indicating that the Ca-O existed in the form of octahedral structure.

$$CN_{ij} = 4\pi\rho_j \int_0^r g_{ij}(r)r^2 dr \quad \text{Equation (2)}$$

The average Sr-O CN was calculated as shown in Fig. 4. Considering a cut-off radius of 3.35 Å for the first coordination shell according to the study of Xiang et al. [71], the average Sr-O CN was about 7.0. Meanwhile, the length of the Sr-O bonds and the Sr-O CN were in good agreement with the study of Xiang et al. [71]. However, due to the larger atomic radius of Sr compared to Ca, the Sr atoms were likely to interact with more oxygen atoms in the lattice. As a result, the Sr-O CN was expected to be higher than that of Ca-O.

The O-Si-O interbond angle represented the intra-structural angle of the tetrahedral units where the Si atom was at the vertex of the angle. The bond angle distribution (BAD) was calculated in order to study and determine the size of the O-Si-O angle. Moreover, the O-Ca-O and O-Sr-O bond angles, which were the short-range structure angles for the lattice modifiers, were calculated and shown in Fig. 5. After averaging the O-Si-O BAD, this value was approximately equal to 109.4° for all the BGs. The exact values are given in Table 3. The value of the O-Si-O bond angle was calculated to be 109.47°, 109.5° or 109.0° in the study of Yuan et al.

[72], Ren et al. [73] and Sharma et al. [74], respectively. According to Fig. 5, two peaks at angles of 60.0° and 80.0° were observed for O-Ca-O. Meanwhile, the O-Sr-O curve was similar to O-Ca-O and had two peaks at angles of 60.0° and 80.0°. The probability of the first and second peaks of the O-Ca-O and O-Sr-O curves did not change much with difference in the amount of CaO in the composition of BGs. The higher ratio of the first peak to the second peak in the O-Sr-O BAD compared to O-Ca-O could be attributed to the higher CN of Sr-O compared to Ca-O, since the increase in the CN of Sr-O caused more oxygen atoms in the neighborhood of Sr and caused the oxygen atoms to come closer to each other and the O-Sr-O angle to decrease. In addition, the Ca-O CN was approximately 6, indicating that the formation of CaO₆ unit structures was created and the occurrence of a peak at an angle of approximately 90.0° confirmed this [74]. The change in peak intensity in the O-Sr-O BAD was also observed in the study of Xiang et al. [71], and the angle of two peaks for the O-Ca-O and O-Sr-O BADs was in good agreement with that study, too [71]. The values of the O-Ca-O BAD angles in the study of Christie et al. [75] had two peaks at approximately 90° and 60°. Similarly, two peaks at 60° and 90° were observed for the O-Sr-O bond angle, while the O-Ca-O BAD was in good agreement with the simulations of other BGs [76,77].

The Si-O-Si bond angle was investigated to study the arrangement of the tetrahedra forming the network with respect to each other. In this

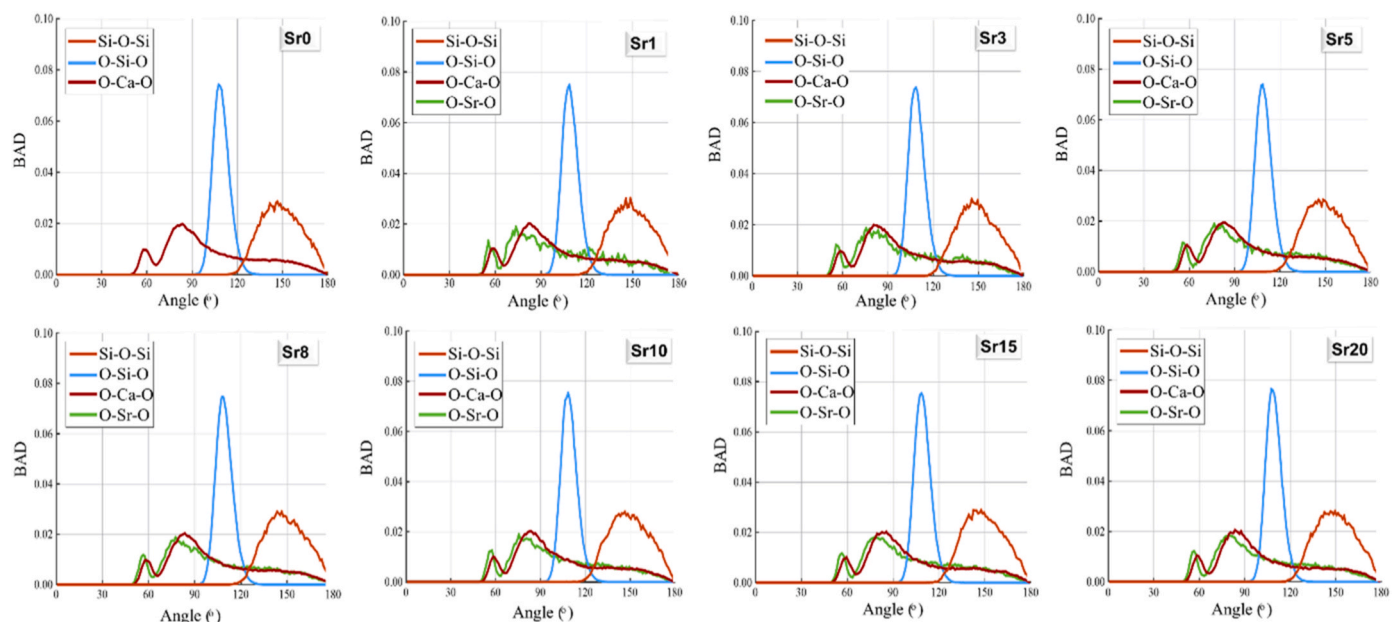


Fig. 5. BAD curves of Sr-doped BGs, for Si-O-Si, O-Si-O, O-Ca-O, and O-Sr-O bonds.

case, the oxygen atom was at the apex of the angle, establishing the connection between 2 Si atoms, known as bridging oxygen (BO). For an oxygen atom only attached to one Si, non-bridging oxygen (NBO) can be observed. The distribution of the Si-O-Si bond angle is displayed in Fig. 5 and the average Si-O-Si bond angles are shown in Table 3. According to these results, the value of the Si-O-Si bond angle in the BGs was in the range of 148.0° to 150.0°. The addition of SrO to the chemical composition of BGs caused the tetrahedra forming the network to be arranged with a wider angle of about 3.0° with respect to each other. This could be due to the introduction of Sr near the network, which, due to the larger atomic radius of Sr compared to Ca, caused the Si-O-Si bond angle to be larger. The value of the Si-O-Si bond angle obtained in this simulation was in good agreement with the results of previous studies [72,78].

3.2. Density and medium-range structure

Fig. 6a shows the change in density with different SrO content. According to the results, the density of BGs progressively increased with the increasing substitution of SrO for CaO. This was due to the higher molar mass of Sr compared to Ca atom and, since the atomic radius of Sr was slightly different from Ca, it caused just a very small change in the volume of BG structure; thus, the increase in mass overcame the increase in volume and the density increased.

Examining network connectivity (NC) and calculating structural parameters between domains can help predict the properties of BGs. Among these parameters, the Q^n distribution, BOs, NBOs, and NC can be mentioned. According to the report by Tilocca [79], BGs with $NC < 3$ can have proper bioactivity and, as a result, higher ion release properties. Fig. 6b shows the distribution of BOs and NBOs in the structure of BGs. According to Fig. 6b, the results indicate that with higher SrO content in the composition, a reduction in the distribution of BOs occurs, while the distribution of NBOs increases. It was also observed that the distribution of free oxygens (oxygen atoms that are not connected to the silicate network) decreased as SrO content increased. This behavior causes

the network-modifying cations to interact only with the oxygens within the network, thereby resulting in a reduction in NC. To study the medium-range structure of BGs, the Q^n distribution was examined (Fig. 6c). Based on the obtained results, it can be observed that the Q^4 and Q^1 species in the structure decreased simultaneously with increasingly higher SrO content, whereas the fraction of Q^2 shows an increase of 1%. Moreover, Q^3 exhibits the highest distribution among the Q^n species, and its proportion also increases with higher SrO content. Using Eq. (3) [80], NC values are calculated and reported in Table 4. The theoretical NC is also calculated using Eq. (4) being equal to around 2.66 for all BGs [81]. The obtained results presented good agreement with the theoretical equation (Fig. 6d).

$$NC = \sum_{n=1}^4 Q^n \cdot n \quad \text{Equation (3)}$$

$$\text{Theoretical NC} = 2 + \frac{2 \times (\text{SiO}_2 - \text{CaO} - \text{SrO})}{\text{SiO}_2} \quad \text{Equation (4)}$$

The obtained results from the NC evaluation indicated that, with increasing the SrO content in the chemical composition of BGs, the NC value tends to decrease. This suggests that SrO can modify the glass network to a greater extent than CaO, thereby increasing the glass degradability. This behavior can be attributed to the higher coordination of Sr-O species: Sr atoms can coordinate a larger number of oxygen atoms compared with Ca, which reduces the formation of BOs, hence reducing the NC. Additionally, it was observed that the NC derived from Eq. (3) was slightly higher than the theoretical values. Meanwhile, considering the distribution of oxygens, it can be seen that if the distribution of free oxygens (oxygen atoms that are not connected to the silicate network) was increased, NC also increases. In addition, the free oxygens in this simulation were oxygens forming Ca-O-Ca bonds, causing fewer network bonds to be broken and, as a result, higher NCs were acquired.

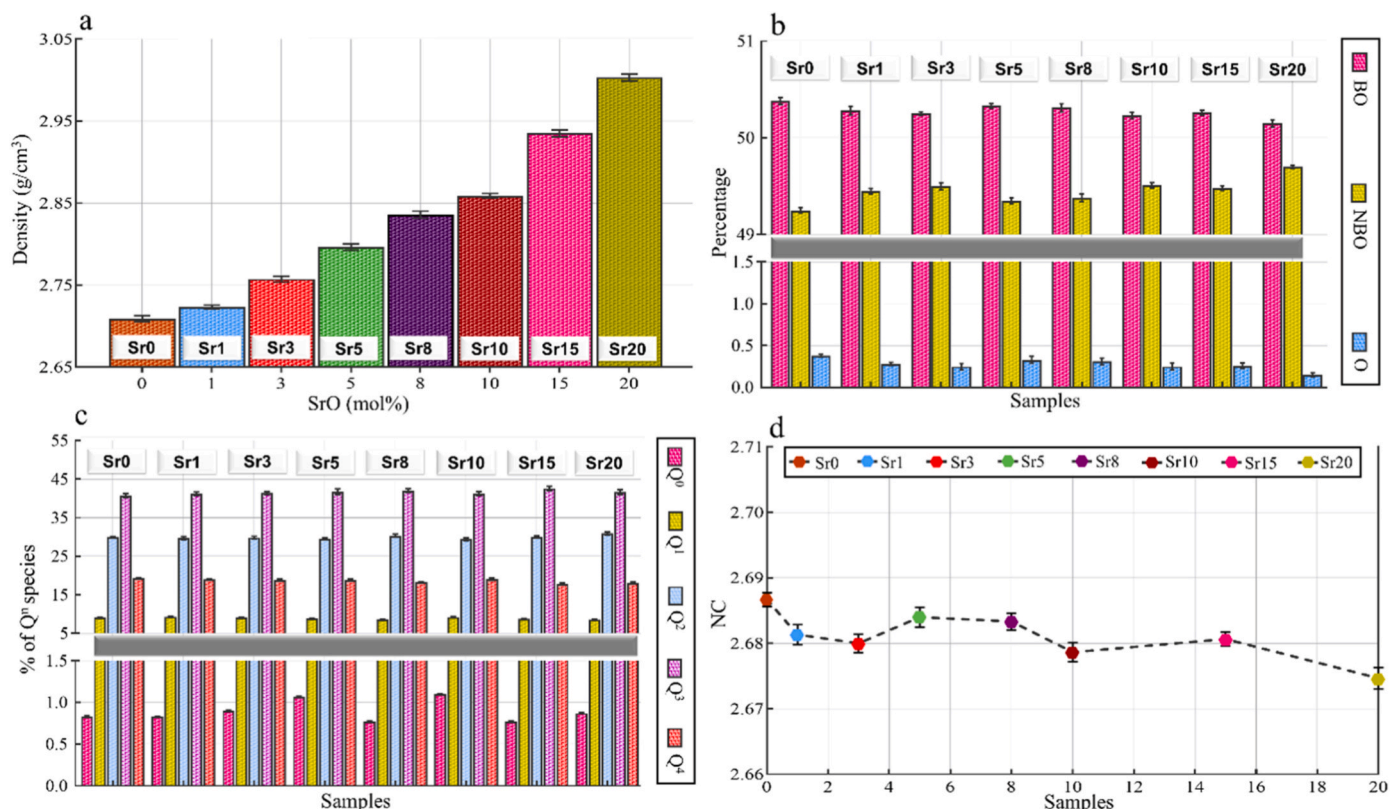


Fig. 6. Sr-doped BGs, a) Density, b) Oxygen bonding types, c) Q^n distribution, and d) Network connectivity.

Table 4
Qⁿ distribution, oxygen types, and network connectivity of simulated BGs.

BGs	Q ⁰ (%)	Q ¹ (%)	Q ² (%)	Q ³ (%)	Q ⁴ (%)	NC	BO (%)	NBO (%)	Free Oxygens (%)
Sr0	0.83 ± 0.0085	9.13 ± 0.0738	29.90 ± 0.2315	40.80 ± 0.5231	19.33 ± 0.1284	2.687 ± 0.00106	50.38 ± 0.0356	49.25 ± 0.0281	0.38 ± 0.0149
Sr1	0.83 ± 0.0049	9.30 ± 0.0921	29.73 ± 0.418	41.17 ± 0.4965	18.97 ± 0.1973	2.681 ± 0.00153	50.28 ± 0.0424	49.45 ± 0.0263	0.28 ± 0.0179
Sr3	0.90 ± 0.0075	9.10 ± 0.0629	29.87 ± 0.2953	41.37 ± 0.3648	18.77 ± 0.3064	2.680 ± 0.00138	50.25 ± 0.0198	49.50 ± 0.0357	0.25 ± 0.0363
Sr5	1.07 ± 0.0039	8.87 ± 0.0841	29.50 ± 0.2846	41.73 ± 0.7102	18.83 ± 0.2635	2.684 ± 0.00152	50.33 ± 0.0226	49.35 ± 0.0294	0.33 ± 0.0421
Sr8	0.77 ± 0.0072	8.63 ± 0.0694	30.33 ± 0.3769	42.03 ± 0.4624	18.23 ± 0.1995	2.683 ± 0.00129	50.31 ± 0.0411	49.38 ± 0.0388	0.31 ± 0.0375
Sr10	1.10 ± 0.0067	9.23 ± 0.0972	29.40 ± 0.4118	41.23 ± 0.5812	19.03 ± 0.3168	2.679 ± 0.00148	50.23 ± 0.0319	49.51 ± 0.0274	0.25 ± 0.0392
Sr15	0.77 ± 0.0086	8.73 ± 0.0763	30.03 ± 0.2912	42.60 ± 0.5639	17.87 ± 0.2416	2.681 ± 0.00108	50.26 ± 0.0263	49.48 ± 0.0241	0.26 ± 0.0326
Sr20	0.87 ± 0.0082	8.53 ± 0.0795	30.93 ± 0.3816	41.60 ± 0.6351	18.07 ± 0.2375	2.675 ± 0.00162	50.15 ± 0.0365	49.70 ± 0.0185	0.15 ± 0.0221

3.3. CNN results

The RSD and RDF calculations were performed based on the prepared code. In this research, the simple and practical method of RDF was used, despite the shortcomings of this function to calculate the ring size distribution. As shown in Fig. 7, the RDF was used to convert the 3D atomic positions to a 2D 10×100 matrix, reducing the order of input data by 1, making it suitable for a 2D CNN network.

Finally, the dataset was prepared as eight 10×100 matrices for the input data Fig. 8a, and eight 1×12 matrices for the target data Fig. 8b.

Overall, the results highlighted the model capability to accurately predict the RSD from RDF. A visual comparison of the predicted and actual RSDs is presented in Fig. 9. The plot displays the predicted values alongside the actual values for ring sizes 1 to 12. The close alignment between the two curves demonstrated the model effectiveness, with only minor deviations observed for certain ring sizes. The performance metrics, evaluated using a rigorous leave-one-out cross-validation (LOOCV) strategy, were annotated in a textbox on the plot. The model achieved a mean MSE of 113.69 ± 34.30 , indicating close agreement between predicted and actual values. Furthermore, a mean R² value of 0.9740 ± 0.0070 demonstrated that the model captures nearly all the variability in the data. The mean correlation coefficient of 0.9899 ± 0.0023 further confirmed a strong linear relationship between predictions and observations. This demonstrates the potential of the approach used, suggesting that even further generalization could be achieved by incorporating additional data.

4. Conclusions

In this study, a combination of MD simulation and deep learning CNN algorithms was used to accurately analyze the structure of Sr-substituted melt-derived silicate-based BGs. Focusing on the composition of the 60SiO₂–(40–x)CaO–xSrO oxide system and its doping with different amounts of SrO, the effect of this compositional change on the short- and medium-range structure, bonding properties, bond angles, and finally the accurate prediction of the RSD was investigated. From the perspective of the short-range structure, the obtained results showed that the SiO₄ structure remained stable in the tetrahedral form and the Si-O CN remained constant at 4 for all compositions. With the increase in the Sr percentage, the Sr-O bond length changed from about 2.56 to 2.60 Å and its CN decreased from 7.25 to 6.89. Moreover, the O-Si-O angle remained at about 109.36° in all samples, which was consistent with the ideal tetrahedral geometry (109.5°), but the Si-O-Si angle increased from the initial value of 148.97° to a maximum of 149.65° due to Sr doping, indicating a more open BG lattice structure and a potential for improved ion exchange ability.

In the medium-range structure, very slight changes were observed by examining the distribution of Qⁿ units, and in most compounds, the ratio of Q³ and Q² was dominant. The gradual increase in the SrO content led to a decrease in the NC value from 2.687 in the Sr0 sample to 2.675 in the Sr20 sample, which was slightly higher than the theoretical value of 2.66 for the unchanged compounds. This increase in NC was related to the increase in the number of free oxygens in the structure and indicated that the BG structure with the substitution of Sr became slightly more stable and denser in terms of NC. Meanwhile, the investigation of the distribution of BO and NBO showed that their ratio remained almost constant and the BG structure at the medium-range level did not undergo fundamental changes. This stability of the structure in the presence of different SrO contents could be an indication of the high chemical flexibility of silicate-based BGs against doping with bioactive elements.

One of the main innovations of this research was the development and implementation of a model based on a 2D CNN to predict the RSD based only on RDF data. Unlike conventional methods based on direct processing of 3D atomic positions, this method was able to extract complex structural patterns and reconstruct the RSD distribution with

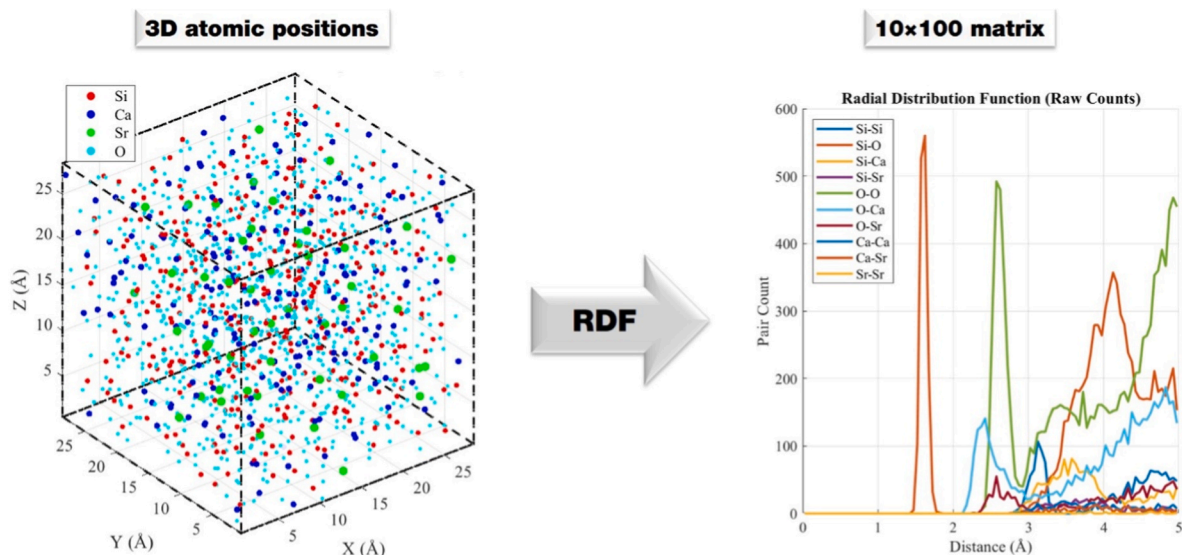


Fig. 7. Input conversion using RDF.

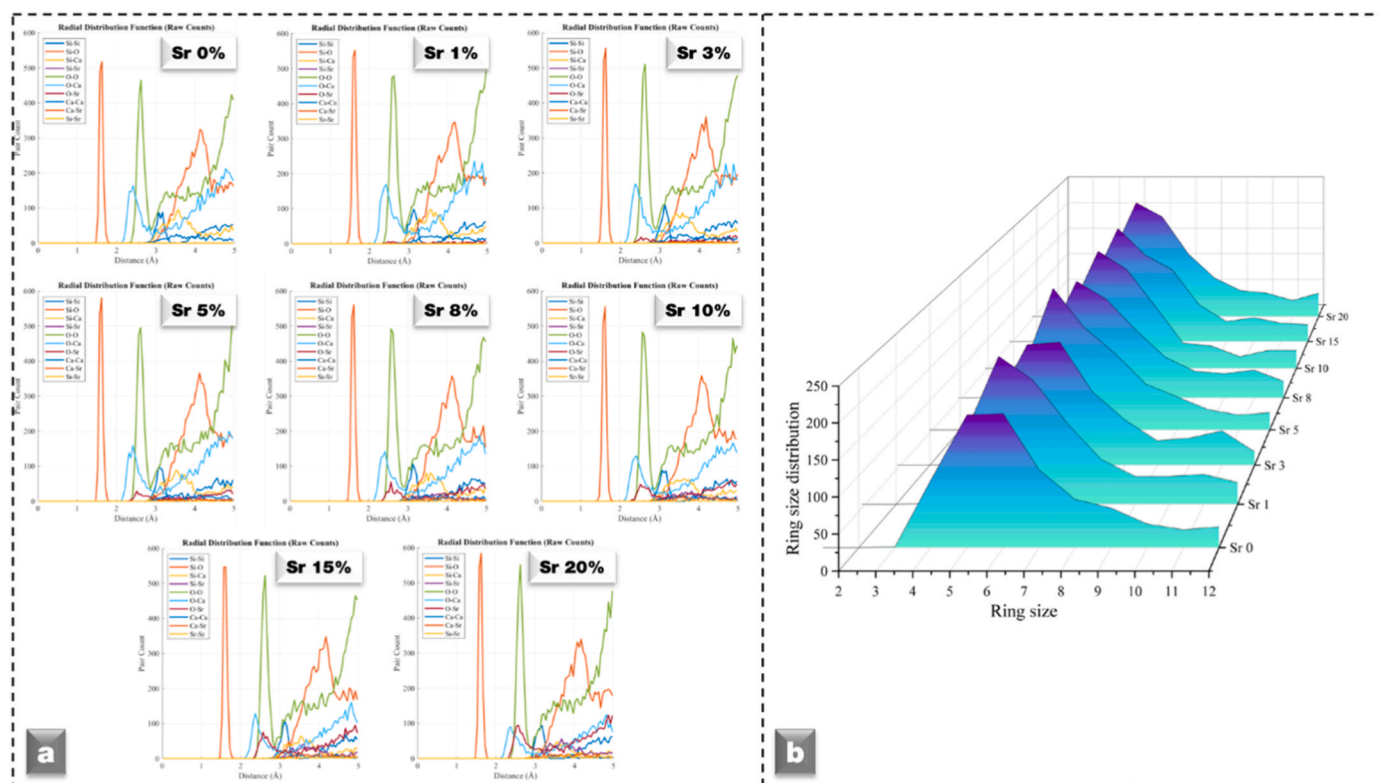


Fig. 8. Prepared dataset for the CNN network, a) input data, b) target data.

acceptable accuracy by reducing the data dimension (by converting RDF to a 10×100 matrix). Despite training the model on only 7 samples, the prediction results using the LOOCV method, showed that the model had good generalization ability and was able to provide a high similarity to the actual RSD distribution with low MSE and acceptable R^2 . The medium-to-high correlation coefficient between the predicted and actual data confirmed the accuracy of the model.

These findings not only confirmed the effects of strontium in altering the structural and network properties of BGs, but also indicated the ability of deep learning models to predict complex properties of non-crystalline materials such as BGs. The use of CNN-based models can be

an efficient, fast, and low-cost alternative to traditional structural simulation and analysis methods, allowing to save computational time compared to traditional MD simulations and paving the way for the design of advanced and optimized biomaterials with targeted properties.

CCRediT authorship contribution statement

Amirhossein Moghanian: Conceptualization, Investigation, Methodology, Project administration, Writing – original draft, Writing – review & editing. **Francesco Baino:** Conceptualization, Data curation, Investigation, Methodology, Writing – original draft, Writing – review &

LOO-CV: Actual vs Predicted Ring Size Distributions

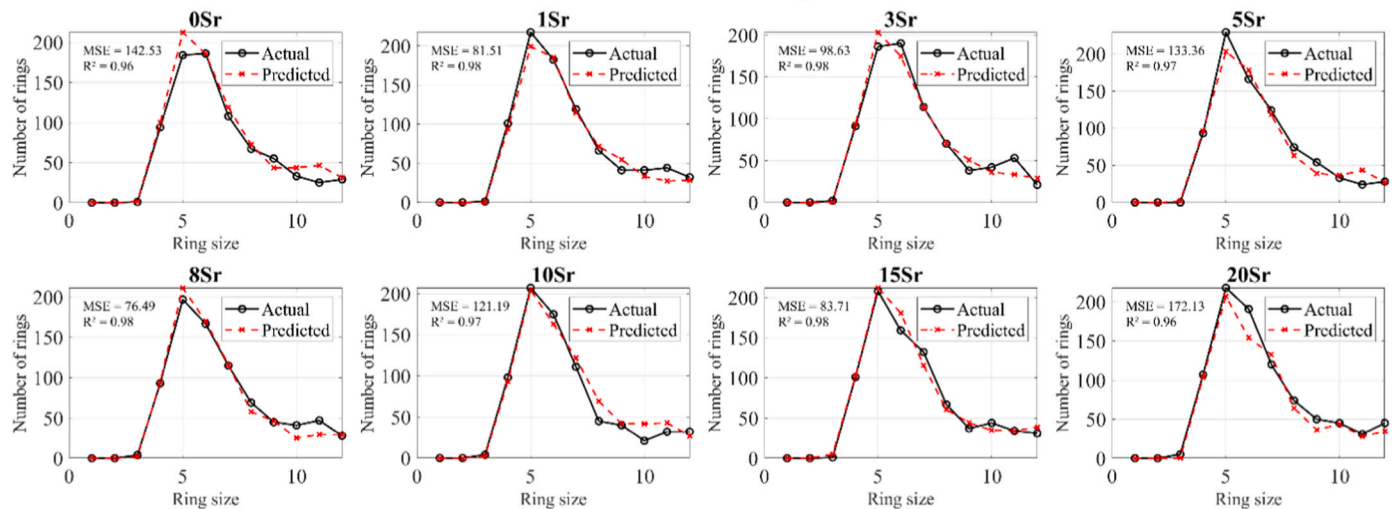


Fig. 9. Predicted values vs. actual values of ring size distribution for all samples using LOOCV.

editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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