Molecular Dynamics-Based Analysis of Cavity Distribution in GeO_2 Glass: A Novel Computational Method

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GeO_2 glass is a material of significant interest due to its applications in optics and microelectronics. Despite its widespread use, the presence and distribution of cavities (voids) within the glass structure remain inadequately understood. This study presents a novel method for calculating and analyzing the distribution of cavities in GeO_2 glass using molecular dynamics simulation data. The approach involves: (1) constructing an atomistic model of GeO_2 glass via molecular dynamics simulations; (2) detecting and quantifying cavities within the glass, including their spatial locations and sizes; and (3) performing statistical analysis to derive the cavity size distribution function. The findings demonstrate that this method effectively determines the size and spatial distribution of cavities in GeO_2 glass. Enhanced understanding of cavity distribution can inform strategies to optimize the optical and structural properties of GeO_2 glass. This cavity calculation method offers a valuable tool for probing the nanoscale architecture of glass materials.

1. Introduction

Amorphous materials such as germanium oxide (GeO_2) and silica (SiO_2) glasses are of considerable interest due to their unique optical, electronic, and mechanical properties [1-3]. These properties are intimately related to the atomic-scale structure and morphology of the glassy network, particularly the presence and distribution of cavities or voids within the material [4-11].

Cavities in glass structures can profoundly influence the material's physical and chemical characteristics. For instance, the size, shape, and connectivity of cavities can affect ion and molecule diffusion rates, alter the efficiency of adsorption processes and catalytic reactions, as well as modify optical transmission and scattering properties [7-15]. Consequently, developing accurate methods to characterize the distribution of cavities in glass networks is essential for understanding and engineering the desired properties of these materials.

While conventional experimental techniques such as positron annihilation spectroscopy, small-angle X-ray scattering, and nitrogen adsorption provide insights into the presence and size of cavities in glasses [7, 15-18], they are limited in their ability to resolve the detailed spatial distribution and connectivity of cavities at the nanoscale. In this study, we propose a data mining approach based on molecular dynamics (MD) simulations to systematically investigate the cavity distribution in GeO_2 glass. MD simulations offer a detailed atomistic representation of the glass structure, which can be utilized to develop a comprehensive cavity analysis methodology. By integrating advanced data processing and statistical analysis techniques, we aim to extract valuable insights into cavity characteristics and their relation to the overall glass network structure. The primary objectives of this study are: (1) to establish a robust computational framework for detecting and quantifying cavities in GeO_2 glass using MD data; (2) to analyze the size distribution, spatial

distribution, and connectivity of the cavities; and (3) to demonstrate the utility of this cavity analysis approach in understanding the structure-property relationships in glass materials.

2. Calculation method

In this study, we analyzed the cavity distribution in GeO_2 glass using a computational approach grounded in molecular dynamics (MD) simulation data. The key steps of the calculation method are outlined below:

MD Model Construction: A GeO_2 glass model was generated using classical MD simulations, employing the Oeffner-Elliott (OE) interatomic potential. The simulation box comprised 5,499 atoms (1,833 Ge and 3,666 O atoms) with periodic boundary conditions. The system was equilibrated at 5000 K and then gradually cooled to 300 K to obtain the final amorphous glass structure [4, 12, 19-22].

Monte Carlo-Based Cavity Volume Calculation: To quantify the cavity volume fraction and its distribution within the glass network, a Monte Carlo approach was utilized. A total of 1,500,000 random points were uniformly distributed within the MD simulation box. For each point, a determination was made as to whether it resided within a cavity (i.e., a region unoccupied by any atoms). The proportion of points located within cavities provided an estimate of the cavity volume fraction [22-27].

Cavity Detection and Size Distribution Analysis: The spatial distribution and sizes of the cavities were determined using the DBSCAN (Density-Based Spatial Clustering of Applications with Noise) algorithm [23-24]. This algorithm clusters data points that are closely located based on a distance metric and the minimum number of points required to form a cluster. In this study, DBSCAN was applied to the set of random points identified as being within cavities. The algorithm enabled the identification of individual cavities and their respective volumes, allowing for the construction of a cavity size distribution function that offers insights into the statistical characteristics of the cavity network in GeO_2 glass. All calculations and data analyses were performed using custom Python scripts, leveraging scientific computing libraries such as NumPy, SciPy, and scikit-learn.

DBSCAN Parameters: The key parameters for the DBSCAN algorithm are epsilon (eps) and *min_samples*. Epsilon defines the maximum distance between two points for them to be considered as part of the same neighborhood, thereby determining the cluster density. *Min_samples* specifies the minimum number of points required to form a dense region, distinguishing between core points (points with at least min_samples neighbors within epsilon) and border points (points with fewer than *min_samples* neighbors within epsilon) [24, 28].

Visualizing Cavity Distribution: To visualize the distribution of cavities in 3D space, we employed a technique of filling the cavity volumes with small spheres. This approach provides a clear visualization of the cavities' spatial distribution.