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Molecular dynamics investigations of silver diffusion in glass

D. Timpel *, K. Scheerschmidt

Max Planck Institute of Microstructure Physics, Weinberg 2, D 06120 Halle, Germany

Abstract

Ion-exchanged sodium silicate glasses are studied by means of molecular dynamics computer simulations with empirical potentials. The sodium is partly exchanged by silver. This results in the generation of Ag particles after reduction of the Ag ions and subsequent annealing. The theoretical calculations investigate the modification of the glass structure and especially by the diffusion processes and mechanisms. A quantitative analysis of the diffusion is performed by calculating and interpreting the mean square displacement, as well as the velocity autocorrelation functions. The validity of these results is supported by long time simulations. © 1998 Elsevier Science B.V. All rights reserved.

1. Introduction

The investigation of the structure and the properties of metallic precipitates in glass is of particular interest, because it permits a purposeful variation of the physical properties of the system. Nanometer-sized crystalline Ag particles in alkali silicate glasses are generated by sodium–silver ion exchange, thermally activated migration, and subsequent annealing. The changes in the glass coloration, polarisation, and mechanical properties depend on the size, shape, and distribution of the particles in the material. The commercial glass, studied experimentally by X-ray diffraction and extended X-ray absorption fine structure (EXAFS) spectroscopy [1], typically comprises a sodium trisilicate with less than 7% CaO, MgO, and Fe_2O_3. Ag particles, of up to 120 nm in size, are created in the glass after ion exchange and annealing. Based on molecular mechanics and dynamics calculations for silver particles embedded in sodium silicate glasses, the possibilities of high resolution electron microscope (HREM) investigations to visualise the structural modifications due to relaxation were discussed in [2]. Thus HREM micrographs of Ag particles in glass, which result in a modification of the lattice fringe contrast of the precipitate, can be interpreted as a shrinkage of the particles with decreasing particle diameter, which is stronger than expected for free particles [1].

In a previous paper [3], a model of a 30% Na–Ag ion exchanged sodium trisilicate glass was investigated by molecular dynamics (MD) simulations, with improved empirical potentials to study clustering and structural modifications. The resulting glass structure showed fair agreement with the results of EXAFS [1] and nuclear magnetic resonance (NMR) spectroscopy [4,5] and was affected by the ion exchange. The sodium was found to be nonuniformly distributed in the glass structure and the existence of channel-like regions, with increased sodium density, was noted. The distribution of the tetrahedral species, Q_n, with n bridging oxygen atoms around the central Si atom, in the MD simulated system, was shown to be in accordance with a thermodynamic model, taking into account the higher glass transition temperature of the

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* Corresponding author. Tel.: +49-345 558 2911; fax: +49-345 558 2917; e-mail: timpel@rmpi-halle.mpg.de.

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simulated system [3,6]. Only for higher ion exchange percentages (80%) was the Q_n distribution affected by the Na–Ag ion exchange. The silver was found to build up a local environment, which is mainly determined by nonbridging oxygen atoms and deviates from the sodium environment. Furthermore, a clustering of the exchanged Ag atoms was observed, depending on the maximum annealing temperature and the Ag–glass interaction. The resulting structural data were used to refine the empirical potentials and the parameters of the Ag–glass interactions. Finally, based on the improved glass models, crystalline Ag precipitates were generated within extended glass structures to improve the HREM image calculations [2,3,6].

In the present paper, the diffusion process itself and the diffusion mechanisms are treated in detail. This information supplements the previous cluster studies [3,6] and gives a comprehensive description of the dynamical properties of the Ag-particle/glass system (diffusion coefficient, vibrational behaviour and migration trajectories).

2. Computational procedure

2.1. Molecular dynamics simulations

To study extended multi-component structures and their long-time dynamical behaviour, it is only possible to employ classical MD with empirical and semiempirical potentials. The MD simulation starts with crystalline structures for disilicates, or with suitable stoichiometric modifications for trisilicates [3,6], and Boltzmann distributed particle velocities appropriate to the initial temperature. The numerical integration of the equations of motion reflects the dynamics of the system.

As in the previous work [3], the MD calculations were performed with constant particle numbers, N, and periodic boundary conditions in all directions. The classical $3N$ Newtonian equations of motion were integrated with an integration step of 1 fs. In order to control the system temperature and pressure, the particle velocities and positions, as well as the dimensions of the simulation cell, were slightly rescaled each time step [7]. The MD simulations are extended to a longer simulation time of 1 ns, to reflect both the diffusion and clustering of the silver atoms over a larger time scale.

The precise physical description of all of the system properties would require the application of quantum mechanics. This, however, is very computer intensive and is limited to systems of about 100 atoms. Thus, for describing a silicate glass structure or metals, semiempirical interaction potentials are employed which are well established and proven [8–13]. In the present paper, a modified Born–Mayer–Huggins (BMH) potential with a three-body Stillinger–Weber term [14,15] and the embedded atomic method (EAM) potential [16] are used to describe the sodium silicate glass and the silver, respectively. The silver–glass interaction, however, for which there are no reported reliable potentials and potential parameters, is described using a modified BMH potential and the refined parameters from Refs. [3,6].

2.2. Simulations

The simulations, based on a sodium trisilicate glass with 1536 atoms, were carried out at constant pressure ($p = 5$ GPa). The sodium–silver ion exchange in the relaxed model was modelled by randomly replacing 30% (in some cases 40–80%) of the sodium atoms by silver at 0 K. The ion-exchanged systems were simulated following annealing for 100 ps at varying temperatures.

For the calculation of the mean square displacement (MSD) and the velocity autocorrelation (VAC) functions, the atomic trajectories were determined at constant temperatures of 300–3000 K, in steps of 300 K. The systems were simulated for 30 ps at constant temperature. When the systems had effectively reached an equilibrium state, the calculations were continued for 12 ps/30 ps at constant volume to evaluate the MSD function, which was calculated at every fifth time step. To obtain additional information about the MSD function, as well as the silver clustering, selected systems were simulated at a constant temperature of 1 ns.

3. Results

The dynamical behaviour of the particles in the glass, i.e. the migration and clustering processes, determine the equilibrium structure and the physical properties of the combined system. Therefore, the diffusion, the diffusion mechanism and the formation of the Ag clusters were analysed in more detail. For the calculation of the dynamical properties, the trajectories were stored every 5 fs. Based on these trajectories, thermal transport coefficients, such as diffusion coefficients, can be evaluated by considering time correlation functions. For this, either the Green–Kubo formula (see standard textbooks, e.g. Ref. [17]) is employed, in which the velocity autocorrelation (VAC) function is integrated over time, or the Einstein relationship can be used, where the mean square displacement (MSD) function is differentiated with respect to time. Transport coefficients are equilibrium properties. Therefore, reasonable results can be only obtained if the system has reached a sufficiently good equilibrium.

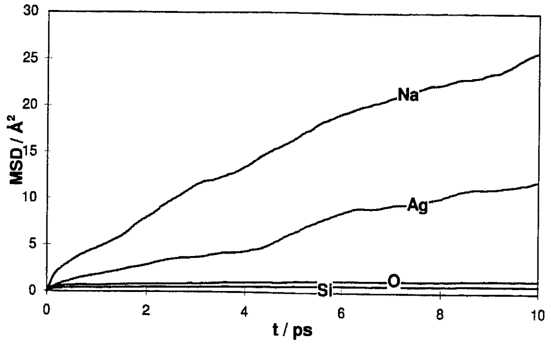

Fig. 1. Mean square displacement for all of the atomic species in a 30% Na–Ag ion exchanged sodium trisilicate glass simulated at $T = 2700$ K.

3.1. Diffusion

The MSD functions for all of the atomic constituents of an ion-exchanged glass at 2700 K are shown in Fig. 1. For Si and O, this function shows only a very slight slope, indicating the lack of any significant diffusion. For these atoms, the MSD values are mainly the result of thermal vibration. Na and Ag, however, show a clearly detectable slope, which allows the calculation of the diffusion coefficients D according to the Einstein relationship (e.g. Ref. [17]):

$$\langle r^2 \rangle = 6Dt + C. \tag{1}$$

In solids, it has been proposed that the diffusion depends on the temperature according to an Arrhenius relationship (e.g. Ref. [18]),

$$D = D_0 e^{-W_{act}/kT}, \tag{2}$$

where W_{act} is the activation energy and D_0 is the diffusion prefactor. Fig. 2 represents the diffusion coefficients for an ion-exchanged sodium trisilicate at temperatures from 300 to 3000 K as an Arrhenius plot. Only for temperatures above 900–1200 K do the diffusion plots for Na and Ag reveal an approximate linearity, consistent with the

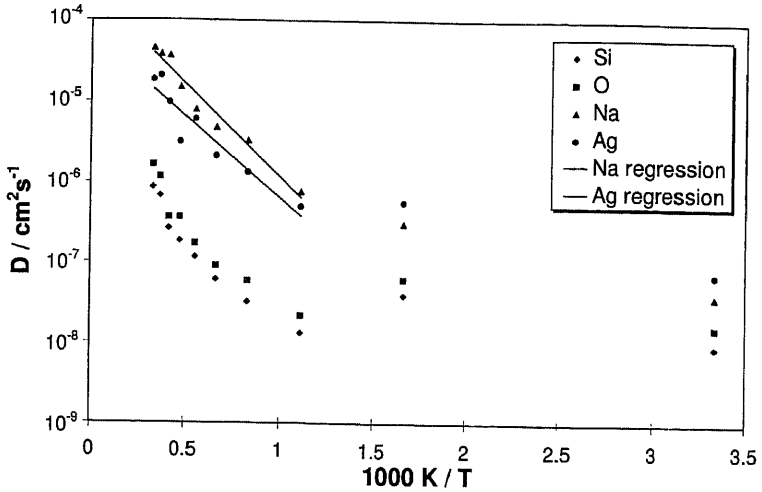

Fig. 2. Simulated diffusion coefficients for a 30% Na–Ag ion exchanged sodium trisilicate glass (straight lines: Arrhenius fit).

Table 1
Comparison of the simulated and experimental activation energies and diffusion prefactors for Na and Ag diffusion in sodium trisilicate glass and 30% Na–Ag ion exchanged sodium trisilicate glass

	W_{Act}(Na) (kJ/mol)	D_0(Na) (cm^2/s)	W_{Act}(Ag) (kJ/mol)	D_0(Ag) (cm^2/s)
Sodium trisilicate glass				
Simul. ($T > 900$ K)	52.0 ± 5.7	$5.60(+2.52-1.74)\times10^{-4}$	–	–
Simul. ($T > 1200$ K)	66.8 ± 2.4	$1.21(+0.18-0.16)\times10^{-3}$	–	–
Expt. [18], (F24)	69.5	1.9×10^{-3}	–	–
Expt. [18], (T1,T8)	70.8	2.63×10^{-3}	–	–
Expt. [18], (M14)	80.4	2.1×10^{-2}	–	–
Expt. [18], (F22)	64.5	8.19×10^{-4}	–	–
Expt. [18], (M13)	63.6	7.9×10^{-4}	–	–
Sodium trisilicate glass (30% Na → Ag)				
Simul. ($T > 900$ K)	48.3 ± 6.1	$2.93(+1.45-0.97)\times10^{-4}$	45.6 ± 9.0	$9.86(+7.96-4.40)\times10^{-5}$
Simul. ($T > 1200$ K)	61.6 ± 6.4	$5.85(+2.62-1.81)\times10^{-4}$	55.2 ± 14.5	$1.63(+2.15-0.93)\times10^{-4}$

temperature dependence of Eq. (2). A linear regression analysis of this portion of the plots enables the calculation of the activation energy, W_{act}, and the diffusion prefactor, D_0. In the MD simulations, the latter depends on the annealing regime and the assumed interatomic potential.

The diffusion prefactor and the activation energy determined from MD simulations for temperatures above 900 and 1200 K, respectively, are summarised in Table 1. For Na diffusion in glasses, there are a lot of experimental measurements (e.g. Ref. [18]), with which the activation energies and the prefactor for the sodium diffusion found here show a remarkable agreement. Both quantities slightly depend on the percentage of the Na–Ag ion exchange.

For silver, however, there exist only a small number of single diffusion measurements [18–22]. These, moreover, show a large dispersion in value. Fig. 3 compares some experimental values to our different simulations. The large dispersion of the experimental results is probably caused by the measuring process and the glass composition. Nevertheless, neglecting the strongly deviating values by Kreibig [18], the high temperature values for the simulated diffusion (>900 K) are in approximate agreement with the experimental data.

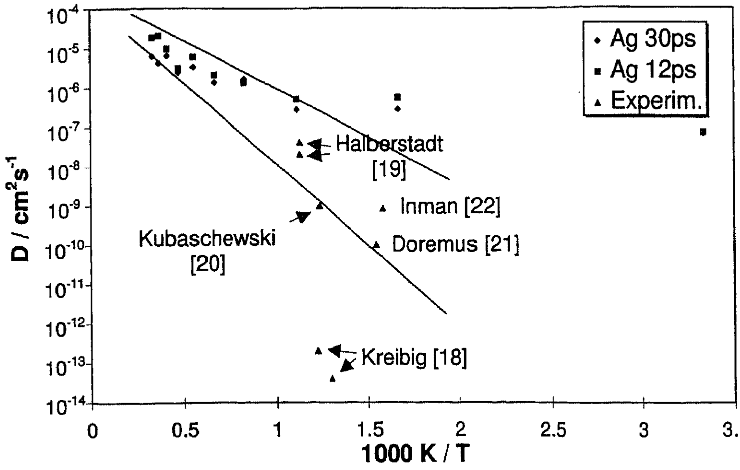

Fig. 3. Comparison of simulated and experimental diffusion coefficients for silver in silicate glasses (straight lines: confidence region).

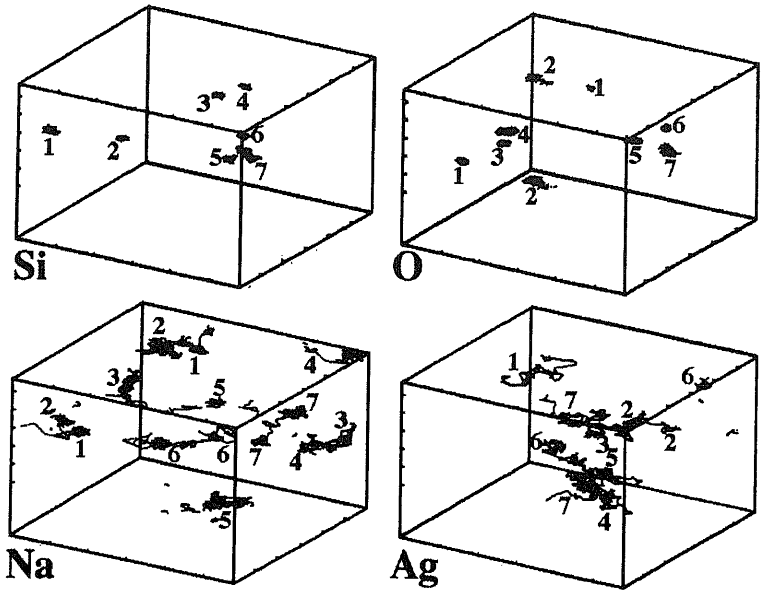

Fig. 4. Trajectory plots for the 7 most mobile Si, O, Na and Ag atoms ($T = 2100$ K; $t = 20$ ps).

3.2. Migration trajectories

The mechanism of diffusion can be clarified by examining the trajectory plots for a 10 ps simulation of an ion exchanged glass matrix at 2400 K (Fig. 4). Only the seven most mobile atoms for each atomic species in the glass are included in this figure, with Si, O, Na, and Ag. Si and O only reveal vibrational movement around a stable site. Within the basic silicate network, the diffusion is negligible. However, the trajectories for Na and Ag partly show long diffusion pathways. These can mostly be separated into two main sections: vibration around stable sites and hops between such sites.

3.3. Vibrational properties

The VAC functions were obtained for all of the atomic species, based on the same trajectories as used to calculate the MSD functions. Fig. 5 shows the first 0.5 ps of the normalised VAC functions for an ion exchanged sodium trisilicate glass at 900 K. The silicon and oxygen VAC functions show a solid-like vibrational behaviour, oscillating with high frequency and rapidly decreasing to approximately zero amplitude. In addition, the VAC functions for Si and O reveal a broad correspondence, indicating a correlation of the Si and O vibrations due to the Si–O bonds. In contrast, the sodium and silver functions decrease slowly which indicates a high translational component in the movement of these atoms.

The VAC function also allows the calculation of the diffusion constant, via the equation (e.g. Ref. [17])

$$D = \frac{1}{3}\int v_0 v(t)\,\mathrm{d}t. \tag{3}$$

The resulting diffusion parameters are in approximate agreement with those calculated from the MSD. The Fourier transformation of the VAC functions results in the vibrational power spectra shown in Fig. 6. The power spectra for Si and O

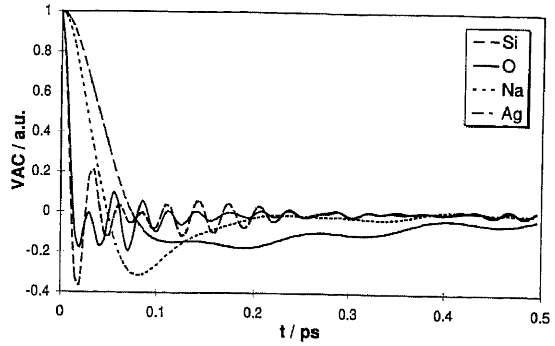

Fig. 5. Normalised velocity autocorrelation functions for a 30% Na–Ag ion exchanged sodium trisilicate glass at $T = 1500$ K.

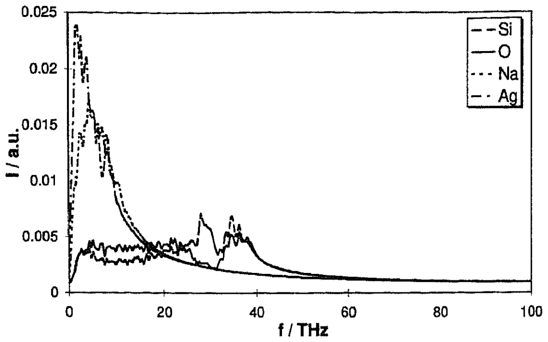

Fig. 6. Fourier transform of the velocity autocorrelation functions in Fig. 5 to yield the corresponding vibrational spectra.

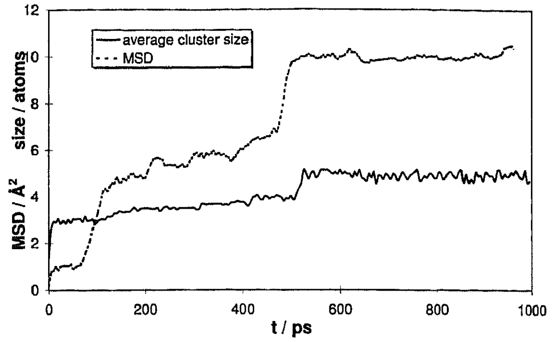

Fig. 7. Comparison of the mean square displacement (in Å^2) and the average cluster size [number of atoms; same scale] for the Ag atoms in a 30% Na–Ag ion exchanged sodium trisilicate glass during a long time simulation of 1 ns.

show a broad band of frequencies (0–40 THz), with distinct peaks at 28 ± 1.5 THz (Si) and 35 ± 1.5 THz (Si, O). The sodium function reveals a pronounced broad peak with its maximum at about 5 ± 2.5 THz. The shape of the Si, O, and Na spectra are only slightly influenced by the presence of Ag. All of the power spectra show a small variation with the temperature. For higher temperatures, the peak maxima are shifted to smaller frequency by about 2 THz.

The vibrational frequencies and mean hopping distance offer a rough estimate of the diffusion prefactor (e.g. Ref. [11])

$$D_0 = \frac{\nu A^2}{6}, \tag{4}$$

where ν is the vibrational frequency, i.e. the attempt frequency for hopping between sites ($\nu_{\mathrm{Na}} \approx 5$ THz, $\nu_{\mathrm{Ag}} \approx 3$ THz) and A is the mean hopping distance, represented by the nearest neighbour distance of the same atomic species (Na–Na, 0.34 nm; Ag–Ag, 0.27 nm). The resulting estimated diffusion prefactors for sodium ($D_{0,\mathrm{Na}} \approx 1.0 \times 10^{-3}$ cm^2 s^{-1}) and silver ($D_{0\,\mathrm{Ag}} \approx 3.6 \times 10^{-4}$ cm^2 s^{-1}) agree fairly well with the values from the MSD calculation.

3.4. Long time simulations

For selected examples, the dynamical behaviour of an ion exchanged glass was studied up to 1 ns. The resulting long time correlations describe the system behaviour on a longer time scale and should enable an evaluation and the correction of the short time diffusion simulations. Silicon and oxygen reveal the same behaviour as already observed for the short simulation times. Also, for temperatures up to 3000 K, their MSD functions do not go beyond 3 Å. However, the sodium diffusion coefficients for the long time simulations are slightly reduced; at high temperatures (1500–3000 K) by a factor of 1.4–1.6 and at lower temperatures (300–1200 K) by a factor of 5–8.

For silver, an evaluation of the long time results seems to be more difficult. In particular, the interaction between the formation of the clusters and the migration of the Ag, which is illustrated in Fig. 7, has to be considered. Here, the MSD function for Ag, as well as the averaged Ag cluster size, is shown for a simulation of 1 ns at 900 K. After a rapid growth during the first 10 ps, the average cluster size slowly increases. This cluster growth is related to the high mobility of the Ag atoms, which in turn is reflected by an increase in the MSD function. The clusters formed, however, obstruct the diffusion process, so that the mean square displacement function increases irregularly. Large steps in the function are probably caused by the decay of smaller clusters. After 500 ps, both functions are roughly constant. This suggests that, at this time, all of the Ag atoms are situated in clusters.

4. Discussion

The simulated values for the Na diffusion, especially for $T > 1200$ K, are in fair agreement with

the experimental results [18]. The long time simulations mainly reveal a decrease in the low temperature diffusion coefficients, which may result in a linearisation of the whole Arrhenius plot of the diffusion for a longer time scale. This seems to justify the assumptions made for the calculation of the activation energy and the diffusion prefactor, i.e. to exclude the low temperature diffusion coefficients.

Silicon and oxygen do not exhibit any diffusion processes at the temperatures (300–3000 K) considered here. Also, at 3000 K and for 1 ns, their MSD functions has not reached 3 Å, indicating only vibrational modes of behaviour. In addition, the analysis of the trajectory plots for Si and O excludes the existence of exchange processes. As stated from recent simulation results [3,6], these facts suggest that the theoretical glass transition temperature for the simulated system is higher than 3000 K.

The silver diffusion shows a rough correlation with experimental results [19–22]. The large dispersion of the experimental values is caused by different experimental techniques and by deviations in the glass composition, which prevent a precise comparison of the experimental and simulated data, as presented for sodium.

5. Conclusions

Our MD-generated model of an ion exchanged sodium trisilicate glass enables the first MD description of the structure and dynamics of silver in a glass. The basic glass structure and the structural modifications caused by the ion exchange, as well as the diffusion and clustering behaviour of the silver atoms, were investigated by means of MD simulations. In contrast to the silicon and oxygen atoms, a strong diffusion through the glass is observed for sodium and silver. Both sodium and silver exhibit similar diffusion mechanisms, discrete hopping between stable sites. The sodium diffusion agrees remarkably well with the experimental values. The results were confirmed by long time simulations of up to 1 ns. An evaluation of the silver diffusion is more difficult, because of the small number of experimental values available. Some of the experiments, however, are in good agreement with our simulations, thus justifying the chosen potentials.

6. Note added in proof

In comparing the ion exchange rates with experiments it should be taken into account that the reduction process of the Ag ions is neglected in the MD simulations.

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