

Using Visualisation Techniques and Molecular Dynamics to Study Atoms Diffusing in Glass

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Abstract

In this poster, virtual reality and visualisation techniques are used to interpret the output of Molecular Dynamics simulations. In particular, mixtures of sodium-disilicate and potassium-silicate are studied. In such systems, the silicon and oxygen atoms form a disordered network. The alkali atoms are relatively mobile and will diffuse through channels in the silica network. This behaviour is rationalised by considering the concept of “accessible free volume”.

Categories and Subject Descriptors (according to ACM CCS): I.3.8 [Computer Graphics]: Applications—

By studying ion transport in alkali silicate glasses through atomistic simulation using Molecular Dynamics [VGM*92, SGG95, SFG*97, GGSW01] we are able to calculate where the individual atoms are at any one moment on the femtosecond to nanosecond time scale. These MD calculations are in good agreement with the structure and dynamics of ion movements in glass known from experimental studies [GS07]. The problem of deciphering cooperative dynamics in these calculations is their inherent complexity, evident not just in stills but also in movies. We show in this poster how surface and volume-based visualisation techniques can be used to depict the spatial relationships between the glass silicate network and the atoms (ions) that are mobile [VGM*92, GGSW01]. In addition, we demonstrate how the cooperative relationships between the mobile ions themselves [SGG95, SFG*97] integrate with the dynamics of the surrounding network.

Constructing isosurfaces around the silica network, coupled with immersive 3D viewing beautifully reveals ion channels penetrating the whole structure that remain morphologically intact over prolonged time sequences [GS07], as shown in Figure 1. The average movement of ions as a function of time is contained in the mean-square displacement (MSD) from an initial position which is illustrated in Figure 2. This separates temporally into three distinct regions, where only the displacement beyond 10 picoseconds contributes to the ionic diffusion. The diffusivity increases with temperature, according to an Arrhenius law. What the time development of the MSD hides, though, is the move-

ment of individual ions which turns out to be quite erratic. Egocentric immersion, however, enables the fastest ions that dominate the average diffusion to be identified “by inspection” using 3D ion tracks and numbering to guide the eye. These form dynamic groups that can then be visualised in movies using isosurfaces to define them (Figure 3). Dynamic atomic activity within glasses is governed by a small number of very mobile “players”, the majority of ions comprising “spectators” which are comparatively stationary.

3D Ion tracks can best be identified using glyphs along the time-course of a cooperative event, identified from immersive observation. These tracks reveal how ions hop into sites previously occupied by other members of the group of “players” within a few picoseconds. This is illustrated in Figure 4, which also includes the rendering of the free volume accessible locally for the cooperative group to operate. Surprisingly the free volume (defined in Figure 4) does not align with the ion track sequence but is approximately orthogonal to the cooperative movement. The source of this extra space relates to local contortions in the conformation of the network. Moreover the dynamics point to mode locking of the neighbouring “spectator” silicons and oxygens to the mobile alkalis at “collective” THz frequencies.

The graphics used here in conjunction with state-of-the-art molecular dynamics calculations are enabling the complexity of atomic migration in glasses to be deciphered quantitatively [GFZC11]. Direct comparisons with global averages obtained empirically are excellent, including the manifestation of correlated dynamics in the stretched exponential

character of the intermediate scattering function. The unique contributions that visualisation techniques make include: (1) identifying cooperative groups in dynamic channels in the silicate network; (2) establishing mode locked behaviour at THz frequencies between mobile members and immobile neighbours; (3) rendering the free volume which locally facilitates the diffusion of atoms along correlated tracks.

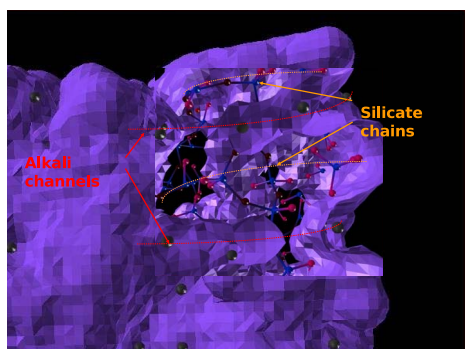


Figure 1: Visualising the spatial relationships between mobile alkali ions and the silicate network in a glass. The isosurfaces (obtained using metaballs) define the zero potential surface between individual alkali atoms and the neighbouring oxygens to which they are chemically bound. This rendering simplifies the complexity of the system to reveal the channels along which alkali atoms diffuse.

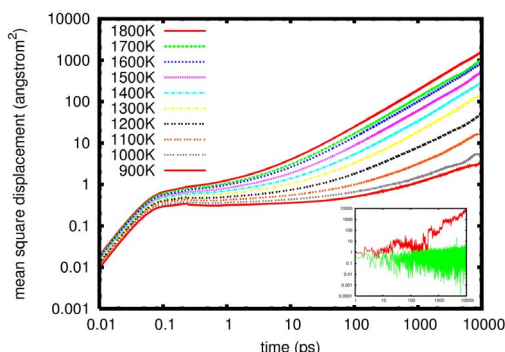


Figure 2: Average mean square displacement (MSD) of sodium ions in a glass as a function of time and temperature, obtained from Molecular Dynamics calculations using DLPoly. Inset shows the movement of individual ions hopping erratically between neighbouring alkali sites but fails to unravel how this happens.

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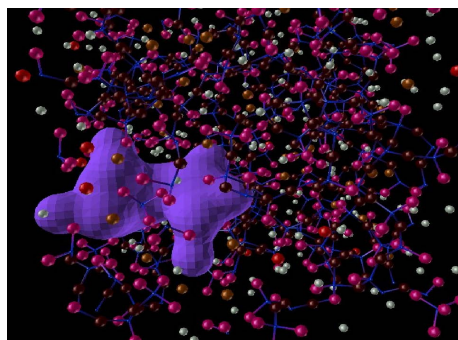


Figure 3: Still from movie showing isosurfaces containing the most mobile ions in a potassium silicate glass. These congregate together and move as a group, simplifying the apparently haphazard individual contributions to the average displacements illustrated in Figure 2.

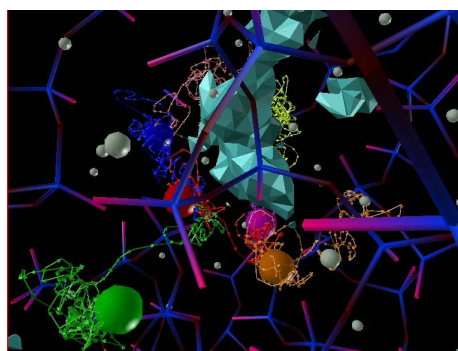


Figure 4: Glyphs used to identify ion tracks in a cooperative event amongst the most mobile ions in a glass, revealing the correlated sequence red, blue, salmon, yellow purple, brown and green. Accessible free volume is bounded by the network isosurface (Figure 1) and the mobile ion isosurface (Figure 3) and can be quantified using the method of marching cubes.

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