Studies of diffusion in ionic glasses on atomic scale

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Ionic glasses are of great interest due to their potential for energy storage solutions, sensor technology or as a way to immobilize nuclear waste over a very long time.

Direct experimental access to processes of atomic diffusion in amorphous solids on the relevant time-scales are very important for the understanding and the quantification of dynamical processes. Atomic scale X-ray Photon Correlation Spectroscopy (aXPCS) provides the necessary experimental access to follow atomic motion in space and time in a model systems of borate glasses with various alkali contents.

We used aXPCS to study diffusion in alkali borate glasses serving as a good example for amorphous ionic conductors [1]. We found for instance [2], that ionic diffusion process as a vacancy mechanism on a network of largely occupied cationic sites strongly decoupled from the slower network dynamics, where alkali ions perform up to 10^9 jumps before the network structure changes, see Fig. 1. While no beam damage is observed, the structural rearrangements indicate instantaneous response proportional to the dose rate. We could associate observed dynamical effects like correlation time length or the shape of the correlation function with various macroscopic properties of glasses like a glass-transition temperature, alkali type and the sample stoichiometry.

Unique possibility of following atomic motion even at room temperature could be seen as a great opportunity to probe various dynamical properties of materials and to study an impact of radiation field on diffusion.

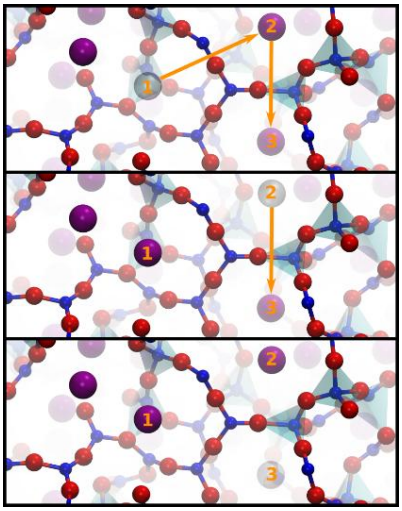

Figure 1: Visualization of the diffusion model by a series of snapshots: large magenta spheres are Rb+ ions, white spheres vacancies, small red circles oxygen and blue are boron atoms. From top to bottom: vacancy makes successive jumps on the three-dimensional arrangement of Rb+ ions.

References

[1] K. Holzweber, C. Tietz, M. Leitner, T.M. Fritz and B. Sepiol, *Beam-induced motion in alkali borate glasses*. Phys. Rev. B **100**, 214305 (2019).

[2] C. Tietz, T.M. Fritz, K. Holzweber, M. Legenstein, B. Sepiol and M. Leitner, *Diffusive dynamics in an amorphous superionic conductor*. Phys. Rev. Research **2**, 043141 (2020).