Local glass structure modification during diffusion views by Raman spectroscopy

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Abstract

Chemical diffusion in amorphous silicates is a process of paramount interest in many different fields including the geosciences, nuclear and industrial glass melting. Indeed, chemical diffusion plays an important role at all stages of the glass melting and transformation process. Recently, the diffusion description in the glass via the eigenvectors and eigenvalues of the full diffusion matrix starts more and more investigated for the different industrial glass systems [1-3]. The advantage of this approach is a possibility to give the general vision of the diffusion process in the explored domain with a limited number of experiments. This macroscopic method lets interpreted the diffusion as exchange reactions that represent the lowest energy pathways that result in material transport and quantify the rate of exchange by eigenvalues. At the same time, spatially-resolved Raman measurements along the diffusion profile showed that less than 20% of vibrations impacted by the diffusion. In this study, to put in evidence the operating microscopic diffusion pathways the Raman spectra has been decomposed on the partial Raman spectra based on NMF approach [4]. Through the comparison of the eigenvalues with the partial spectra contributions we try to associate each partial Raman spectra to one exchange reactions. The analysis of the vibration bands in the partial Raman spectra and they comparison with the literature used here to identify specific structural entities involved in associated exchange reactions.

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