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Article

Suppression of Rayleigh Scattering in Silica Glass by Codoping Boron and Fluorine: Molecular Dynamics Simulations with Force-Matching and Neural Network Potentials

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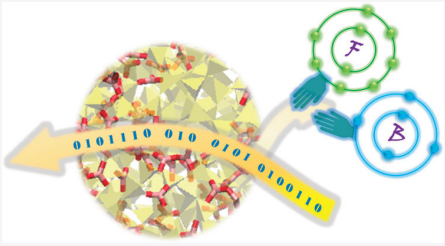
ABSTRACT: Rayleigh scattering attributed to the density fluctuation of silica glass is considered as the intrinsic origin of optical loss in glass fiber. Therefore, minimizing the density fluctuation is key to improving the information and telecommunications networks. In this study, classical molecular dynamics (MD) simulations were employed to theoretically examine the effectiveness of codoping boron and fluorine for ameliorating the homogeneity of silica glass. For the MD simulations, the force-matching potential (FMP) with a Buckingham formula was developed by optimizing the parameters to reproduce the force and energy calculated by the density functional theory (DFT). The accuracy of the FMP was confirmed via comparisons with available experimental data as well as glass models constructed using the neural network potential, which was superior in reproducing the force and energy of the DFT data to the FMP. As a result, the small amount of boron and fluorine added to the silica glass was found not to deteriorate the density fluctuation of silica glass. The additives reduce the viscosity of silica glass, which leads to a lower fictive temperature and, thus, to a better homogeneity. Consequently, the codoping of boron and fluorine was suggested as a possible solution to suppress the Rayleigh scattering of optical glass fiber.



INTRODUCTION

The considerable increase in network communications attributed to the widespread use of mobile devices, Internet of Things, and 5G communication technologies has led to the need for further improvements in traffic speed and capacity.[1,2] Although significant efforts have already been invested to suppress the attenuation of optical communication,[3] the reduction of the optical traffic loss of silica glass-based optical fiber remains an important challenge. A possible method for minimizing the optical traffic loss of the silica glass fiber is doping fluorine[4−11] or sodium[12,13] because such additives reduce the fictive temperature of silica glass, which promotes the homogenization of silica glass. Ono et al. found that pressurized silica glass also increases homogeneity in the nanoscale, and optical loss related to the density fluctuation is suppressed.[14] Further, the density fluctuation of the silica glass fiber is affected by the thermal history of the drawing process, and therefore, the process temperature and the viscosity of the materials are important factors for minimizing the Rayleigh scattering, which causes the optical traffic loss.[15]

Classical molecular dynamics (MD) simulations are useful to understand the effects of pressure and additives on the density fluctuation of silica glass theoretically, instead of time-consuming experiments under such extreme conditions.[16−18] Determining an accurate force field is crucial for the MD simulations to qualitatively examine the effect of the additives. Therefore, in our previous works, the force-matching potential (FMP) was developed by fitting the parameters of a Buckingham formula to reproduce forces and energies calculated by the density functional theory (DFT).[17,18] With the FMP, the effect of fluorine on the reduction of the density fluctuation of the silica glass was well-reproduced.[17] In addition, the codoping effect of Al_2O_3 and fluorine was investigated theoretically. The study suggested that the melting temperature should be sufficiently lowered to reduce the density fluctuation of the Al_2O_3-doped silica glass because Al_2O_3 tends to congregate and, therefore, decrease the homogeneity of the silica glass.[18] In this work, we examine the effect of another dopant, B_2O_3, in minimizing the density fluctuation of the silica glass, as a subsequent study.

Borosilicate (BS) glass is difficult to model using the classical MD simulations due to its complex composition.[19−26] In BS glass with a high B_2O_3 content, boron atoms form sp^2-planar BO_3 units that form a six-membered ring structure called the

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