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RESEARCH ARTICLE

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Theoretical estimation of dielectric loss of oxide glasses using nonequilibrium molecular dynamics simulations

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Abstract

To theoretically explore amorphous materials with a sufficiently low dielectric loss, which are essential for next-generation communication devices, the applicability of a nonequilibrium molecular dynamics simulation employing an external alternating electric field was examined using alkaline silicate glass models. In this method, the dielectric loss is directly evaluated as the phase shift of the dipole moment from the applied electric field. This method enabled us to evaluate the dielectric loss in a wide frequency range from 1 GHz to 10 THz. It was observed that the dielectric loss reaches its maximum at a few THz. The simulation method was found to qualitatively reproduce the effects of alkaline content and alkaline type on the dielectric loss. Furthermore, it reasonably reproduced the effect of mixed alkalines on the dielectric loss, which was observed in our experiments on sodium and/or potassium silicate glasses. Alkaline mixing was thus found to reduce the dielectric loss.

KEYWORDS
dielectric loss, glass, mixed alkaline effect, molecular dynamics

1 | INTRODUCTION

The rapid increase in communication traffic due to the widespread use of the Internet of things, and machine-to-machine and device-to-device communication demands next-generation mobile communication technologies, such as 5G and 6G network systems.[1–5] Such advanced mobile communication systems require solutions for large-capacity transmission, low-latency transport, and ultradense cellular access. A key to increase the transmission capacity and data rate is expanding the communication bands to frequency ranges higher than the 380–5925 MHz range used in conventional network equipment.[1–3] The new band ranges from 6 to 60 GHz, and even higher ones up to 275 GHz would be applied in the coming technologies.[3]

A drawback of the high-frequency radio waves is their short connection range. Therefore, materials used for communication devices should aim to minimize traffic loss. In addition, it is necessary for even the architectural materials to be transparent for radio-wave applications because many devices are used indoors. It is thus important to know the dielectric loss of a variety of materials used to develop next-generation technologies.[6] In terms of glass substrates, considerable effort has been devoted to measure the dielectric loss at the GHz range for developing low-temperature Co-fired ceramics (LTCCs).[7] However, the glassy materials for LTCCs exhibit a low melting temperature and do not include alkalines; these materials are thus not suitable for window and cover glasses. Although Navias and Green reported the dielectric loss for over a hundred types of glasses,[8] data on glass compositions applicable to windows and cover glasses are very limited. Furthermore, most experimental data are limited in a narrow frequency range from 3 and 10 GHz, or even less than MHz range.[9–11] Therefore, theoretical method to

