Electronic Supplementary Material (ESI) for Soft Matter.

Electronic Supplementary Information

Dynamic Behaviour of Water Molecules in Heterogeneous Free Space Formed in an Epoxy Resin

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Contents

1. Glass transition temperature

The glass transition temperature (T_g) was defined as the temperature at which a slope of the relationship between temperature and density changed. The equilibrium density of an epoxy resin was calculated by the simulation for 0.5 ns at each temperature under the NPT ensemble, by lowering the temperature from 500 K to 200 K with a decrement of 10 K. Fig. S1 shows the temperature dependence of density for the 95 %-cured epoxy resin with water contents of (a) 0 wt%, (b) 1 wt%, (c) 2 wt%, (d) 3 wt%, and (e) 4 wt%. In each panel, blue lines were fitted both from the higher and lower temperature sides, and their intersection was defined as the T_g, as indicated by a red arrow.

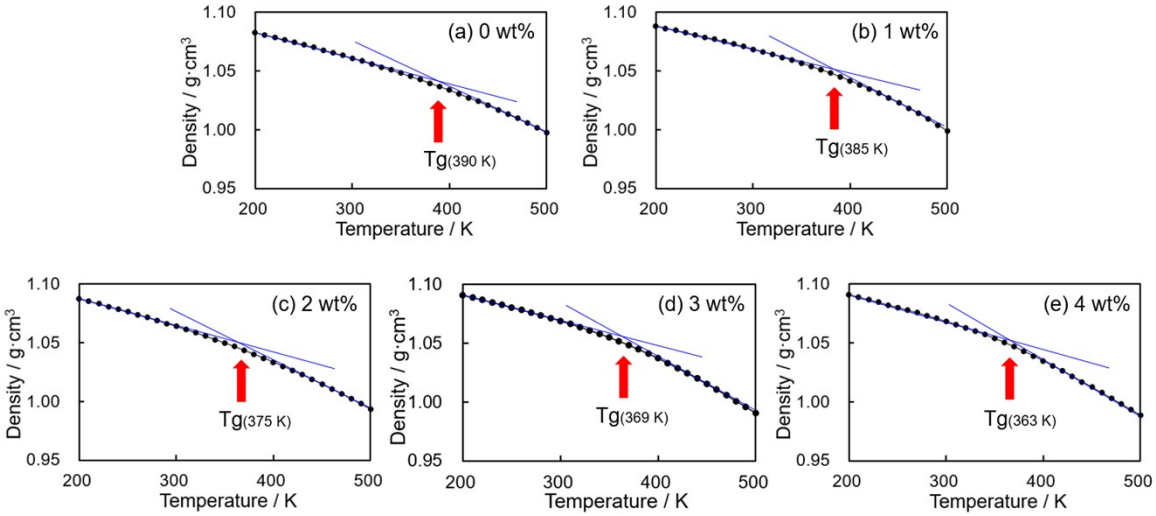

Fig. S1 Relationship between temperature and density for an epoxy resin with water contents of (a) 0 wt%, (b) 1 wt%, (c) 2 wt%, (d) 3 wt%, and (e) 4 wt%.

2. Self-diffusion coefficient

Since the MD simulation for sampling was performed after equilibration, the self-diffusion coefficient of water molecules was analyzed using all 10 ns trajectories. Fig. S2 shows the relationship between time and mean-square-displacement (MSD) of all water molecules in the 95 %-cured epoxy resin with 4 wt% water at 353 K; (a) with and (b) without the electrical charge of water molecules. To ensure the data quality, the MSD data up to a period of 5 ns were used for analysis. The self-diffusion coefficient of water molecules was calculated from the slope of the linear relationship between time and MSD, as guided by a blue line. To obtain the histogram, this operation was sequentially applied for each water molecule.

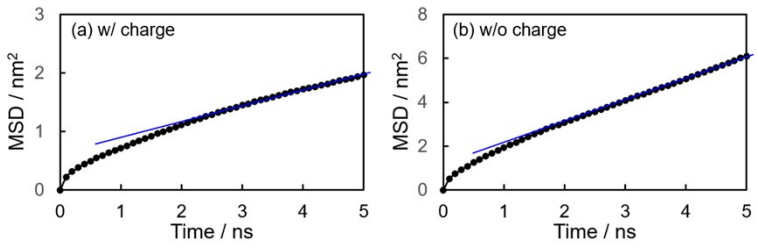

Fig. S2 Relationship between time and mean-square-displacement of water molecules; (a) with and (b) without the electrical charge of water molecules.