Supporting Information

Mechanism of glass transition temperature enhancement in multicomponent epoxy resins incorporating triazine rings

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1 Origin of the low-angle scattering peak

In the WAXS patterns, peak 1 shifts toward lower scattering angles as the TEPIC content increases. This peak has also been observed in single-component epoxy systems, such as DGEBA–diaminodiethylamine [1, 2]. It has been reported that this peak originates from the emergence of periodicity among epoxy monomers or curing agents during curing [3, 4]. To elucidate the origin of peak 1, this study focused on the crosslinked structure of the 0 wt% system without TEPIC. Figure S1 shows the distance distribution between the sulfur atoms of the 4,4'-DDS units bonded to both ends of DGEBA in the 0 wt% formulation. The S-S distance is most frequently distributed around 17–18 Å. Considering that this peak emerges as a result of the curing reaction and that the sulfone group in 4,4'-DDS is expected to have the highest electron density, it is reasonable to attribute this peak to the distance between the sulfur atoms of the 4,4'-DDS molecules connected to both ends of DGEBA. In addition, the apparent shift of this peak toward lower scattering angles with increasing TEPIC content may be attributed to the emergence of an additional peak, originating from structural inhomogeneities observed by DMA or from 4,4'-DDS aggregation. The overlap of this contribution with peak 1 could make the peak position appear to shift.

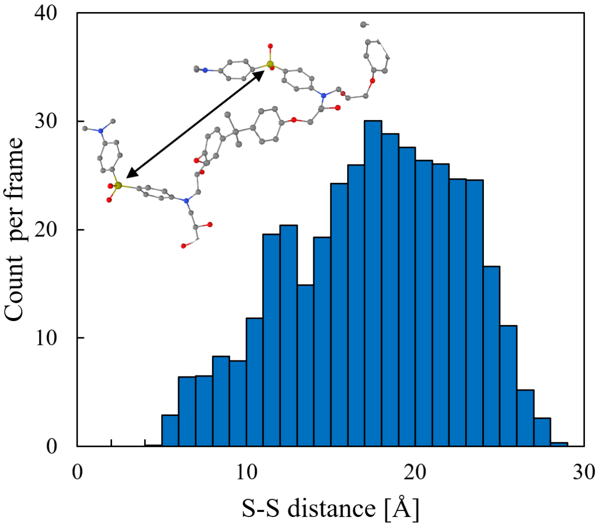
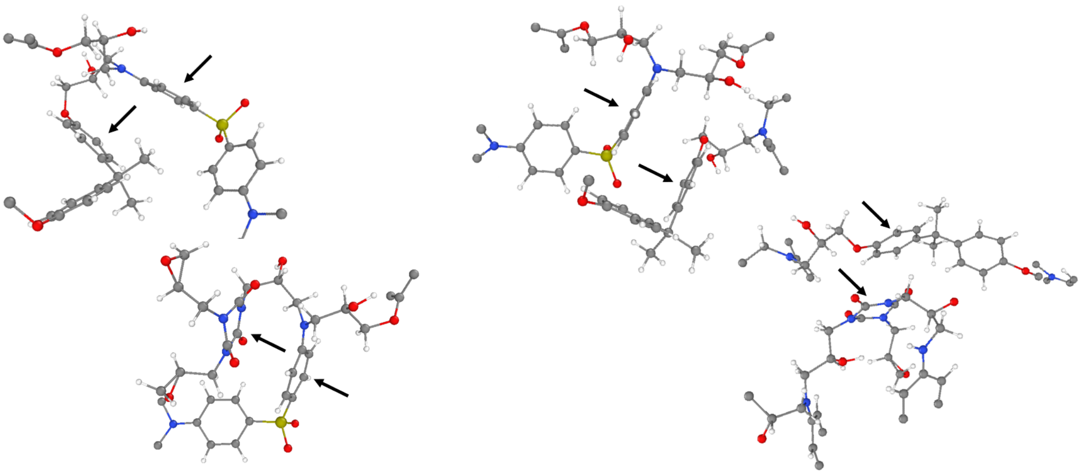


Fig. S1: Distance distribution between the sulfur atoms of the 4,4'-DDS units bonded to both ends of DGEBA in DGEBA/4,4'-DDS

2 Configurations of π–π stacking

Figure S2 shows a visualization of the local ring structures identified as being in a stacked state based on the MD simulations. In both benzene–benzene and benzene–triazine pairs, stacking is observed for both intramolecular and intermolecular configurations. In contrast, the distribution of the center-of-mass distances for stacked pairs shown in Figure 9 does not exhibit a single well-defined peak. This may be because intramolecular and intermolecular stacking experience different constraints and steric hindrance from surrounding atoms, leading to different preferred equilibrium distances, which are superimposed in the observed distribution.

Figure S3 shows the configurations of π–π stacking calculated by quantum-chemical calculations. Benzene–benzene stacking adopts a slipped configuration, whereas benzene–triazine stacking forms a face-to-face configuration.



(a) Intramolecular stacking (b) Intermolecular stacking

Fig. S2: Visualization of stacking configurations determined by MD simulation. C atoms are shown in grey, N atoms in blue, S atoms in yellow, O atoms in red, and H atoms in white. The arrow indicates stacked rings.

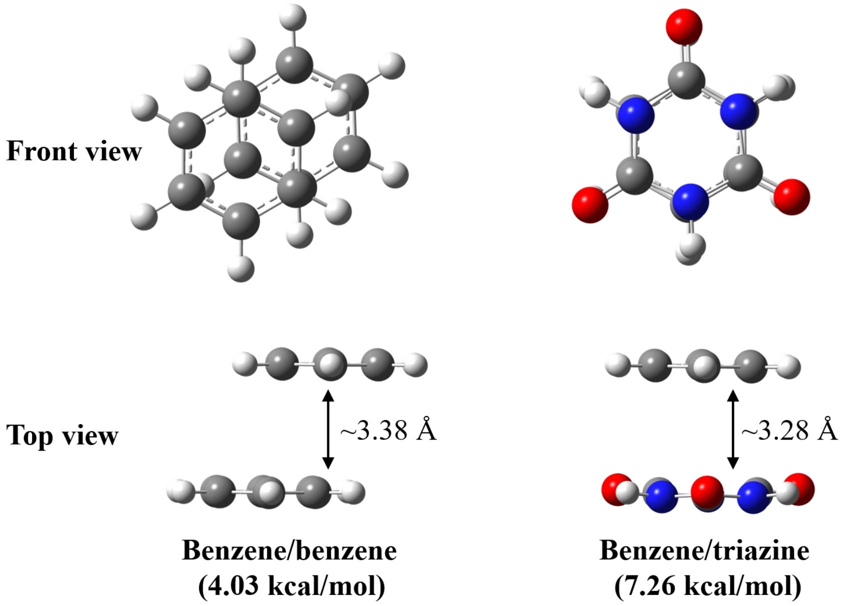


Fig. S3: Configurations of π–π stacking calculated by quantum-chemical calculations.

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