Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary material

Determination of interaction parameters in a bottom-up approach employed in reactive dissipative particle dynamics simulation for thermosetting polymers

Kaiwen Li[1,2], Gota Kikugawa[2]*, Yoshiaki Kawagoe[3], Yinbo Zhao[4] and Tomonaga Okabe[3,5,6]

[1] *Department of Finemechanics, Graduate School of Engineering, Tohoku University, 6-6-01, Aramaki Aza Aoba, Aoba-ku, Sendai,Miyagi, 980-8597, Japan*

[2] *Institute of Fluid Science, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan*

[3] *Department of Aerospace Engineering, Graduate School of Engineering, Tohoku University, 6-6-01, Aramaki Aza Aoba, Aoba-ku, Sendai, Miyagi, 980-8597, Japan*

[4] *School of Aerospace Engineering and Applied Mechanics, Tongji University, Shanghai, 200092, PR China*

[5] *Department of Materials Science and Engineering, University of Washington, BOX 352120, Seattle, WA 98195-1750, USA*

[6] *Research Center for Structural Materials, Polymer Matrix Hybrid Composite Materials Group, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan*

*kikugawa@tohoku.ac.jp

1. DPD interaction parameters for conservative force

This serves as a supplement to the research methods in the main text. The interaction parameter, e_{ij}, between different beads can be calculated by the Hildebrand solubility parameter and Krevelen solubility parameter.

The calculation method has been described in the main text at character 2. The Flory–Huggins parameter is calculated through the solubility parameter and then the interaction parameter e_{ij} can be calculated through the number density of beads and Flory–Huggins parameter. In this study, DGEBA/4,4'-DDS, DGEBA/MPDA and DGEBA/DETA systems have two interaction parameters calculated by Hildebrand solubility parameter and Krevelen solubility parameter. The detailed interaction parameters are listed in the following table.

Table S1 Interaction parameter a in DPD simulation of DGEBA/MPDA system.

e_{ij} (Hildebrand) (10^{-19}(J))	A	B	C	F	G	A’	F’	F’’
A	1.911117							
B	2.160074	2.121711						
C	2.219681	2.735986	2.281532					
F	0.718447	1.262264	0.694192	0.199731				
G	1.790857	2.070201	2.062196	1.698184	1.674881			
A’	1.253929	1.585348	1.445778	1.178192	0.524337	0.808227		
F’	1.808586	2.16237	2.008788	1.66364	0.760512	1.165713	1.674881	
F’’	1.900519	2.321243	2.039603	1.703801	0.821875	1.223451	0.907979	1.787306

e_{ij} (Krevelen) (10^{-19}(J))	A	B	C	F	G	A’	F’	F’’
A	1.448549							
B	2.136896	2.400097						
C	1.616864	2.581433	1.636325					
F	0.803499	1.810491	0.64804	0.246846				
G	1.785837	2.689286	1.880088	2.403104	2.13601			
A’	1.629187	1.784243	2.061803	2.514946	1.419142	1.320121		
F’	1.048548	1.357283	1.360188	1.699336	0.879102	1.006393	0.657773	
F’’	1.503403	2.240103	1.652464	2.119472	0.948394	1.715706	1.167418	1.557178

Table S2 Interaction parameter a in DPD simulation of DGEBA/4'4'-DDS system.

e_{ij} (Hildebrand) (10^{-19}(J))	A	B	C	D	E	A'	D'	D''
A	1.299695							
B	1.678215	2.155754						
C	2.135366	2.336087	1.468592					
D	2.131794	2.526251	1.900348	2.363389				
E	1.072229	1.195685	1.0594	1.121941	0.493322			
A'	1.568609	1.815391	1.418004	1.682192	0.777183	1.184193		
D'	2.4437	2.959243	2.284212	2.851919	1.33658	2.0256	3.44131	
D''	2.733831	3.350331	2.617358	3.279262	1.529103	2.327793	3.957011	4.549987

e_{ij} (Krevelen) (10^{-19}(J))	A	B	C	D	E	A'	D'	D''
A	1.299695							
B	1.977187	2.155754						
C	1.467691	2.447191	1.468592					
D	1.771902	2.402332	2.029133	2.363389				
E	1.743902	1.112505	2.48615	1.604284	0.493322			
A'	1.515187	1.602478	1.978588	1.789104	0.922861	1.184193		
D'	2.127558	2.867455	2.382785	2.852165	1.787064	2.134152	3.44131	
D''	2.476824	3.20168	2.791444	3.285973	1.797296	2.369113	3.958555	4.549987

Table S3 Interaction parameter a in DPD simulation of DGEBA/DETA system.

e_{ij} (Hildebrand) (10^{-19}(J))	A	B	C	H	I	A’	H’	H’’
A	1.682878							
B	1.887813	1.808836						
C	1.934067	2.502893	1.945498					
H	1.284275	1.6818	1.445196	0.973598				
I	1.58677	2.051275	1.690179	1.189693	1.426836			
A’	1.488164	1.835586	1.703357	1.144377	1.404422	1.339324		
H’	1.58677	2.051275	1.690179	1.189693	1.426836	1.007555	1.426836	
H’’	1.603168	1.999685	1.774975	1.218047	1.480666	1.432472	1.480666	1.522937
I’	1.603168	1.999685	1.774975	1.218047	1.480666	1.432472	1.480666	1.522937
e_{ij} (Krevelen) (10^{-19}(J))	A	B	C	H	I	A’	H’	H’’
A	1.373724							
B	2.15122	2.277287						
C	1.460308	2.266346	1.552013					
H	1.182927	1.581824	1.257283	0.893633				
I	1.436684	2.093724	1.528786	1.172515	1.476863			
A’	1.643626	1.696182	1.729902	1.167402	1.569927	1.251791		
H’	1.354554	1.994627	1.441529	1.106796	1.391301	1.569927	1.476863	
H’’	1.784892	2.327671	1.897231	1.385278	1.804045	1.716756	1.804045	2.146535
I’	1.784892	2.327671	1.897231	1.385278	1.701552	1.716756	1.701552	2.146535

2. Equilibrium distance and equilibrium angle for DPD simulation

This part shows the probability distribution of the bond distance and bond angle between atomic groups corresponding to DPD beads in DGEBA/4,4'-DDS, DGEBA/MPDA and DGEBA/DETA system. We got results by searching peaks in these curves.

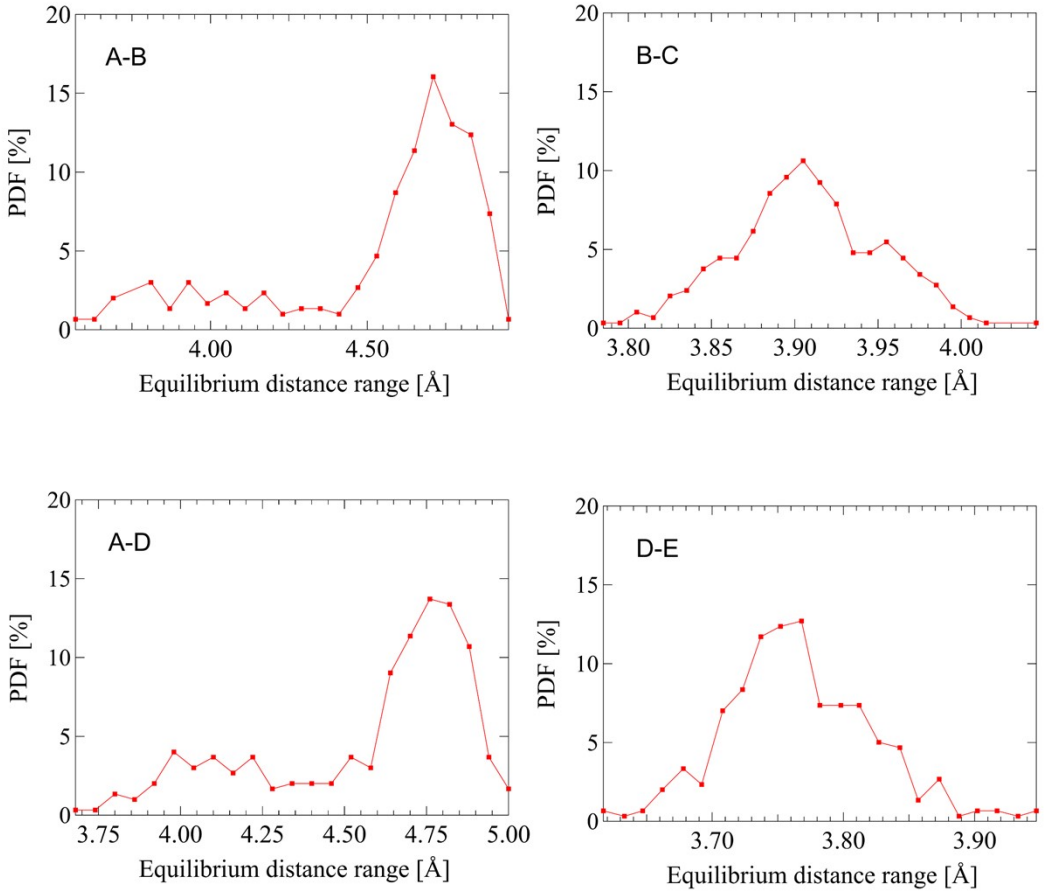

Fig. S1 Probability distribution diagram of the equilibrium distance between bonded beads in the DGEBA/4,4'-DDS system.

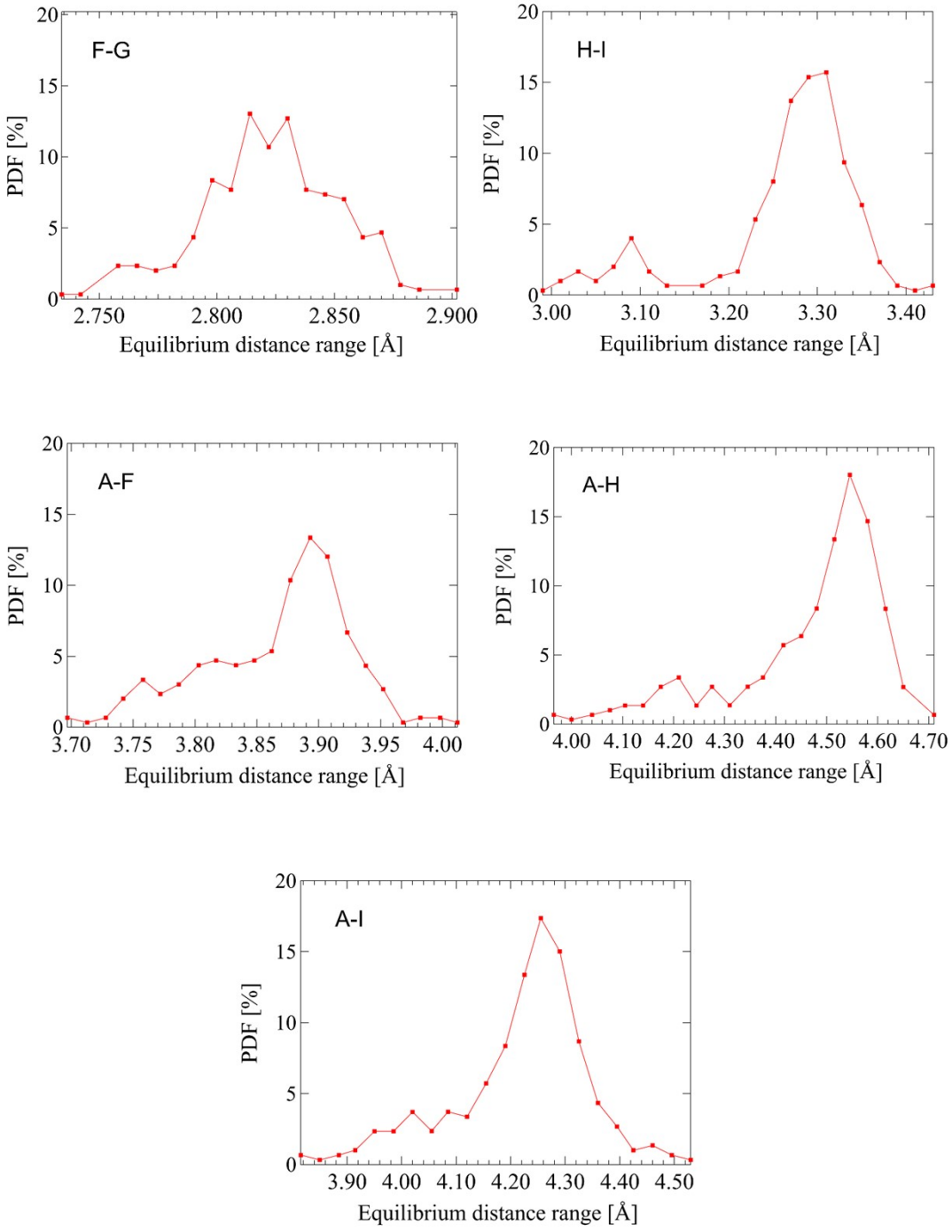

Fig. S2 Equilibrium distance in DGEBA/MPDA and DGEBA/DETA system. DGEBA includes A, B, C beads. MPDA includes F, G beads. DETA includes H, I beads

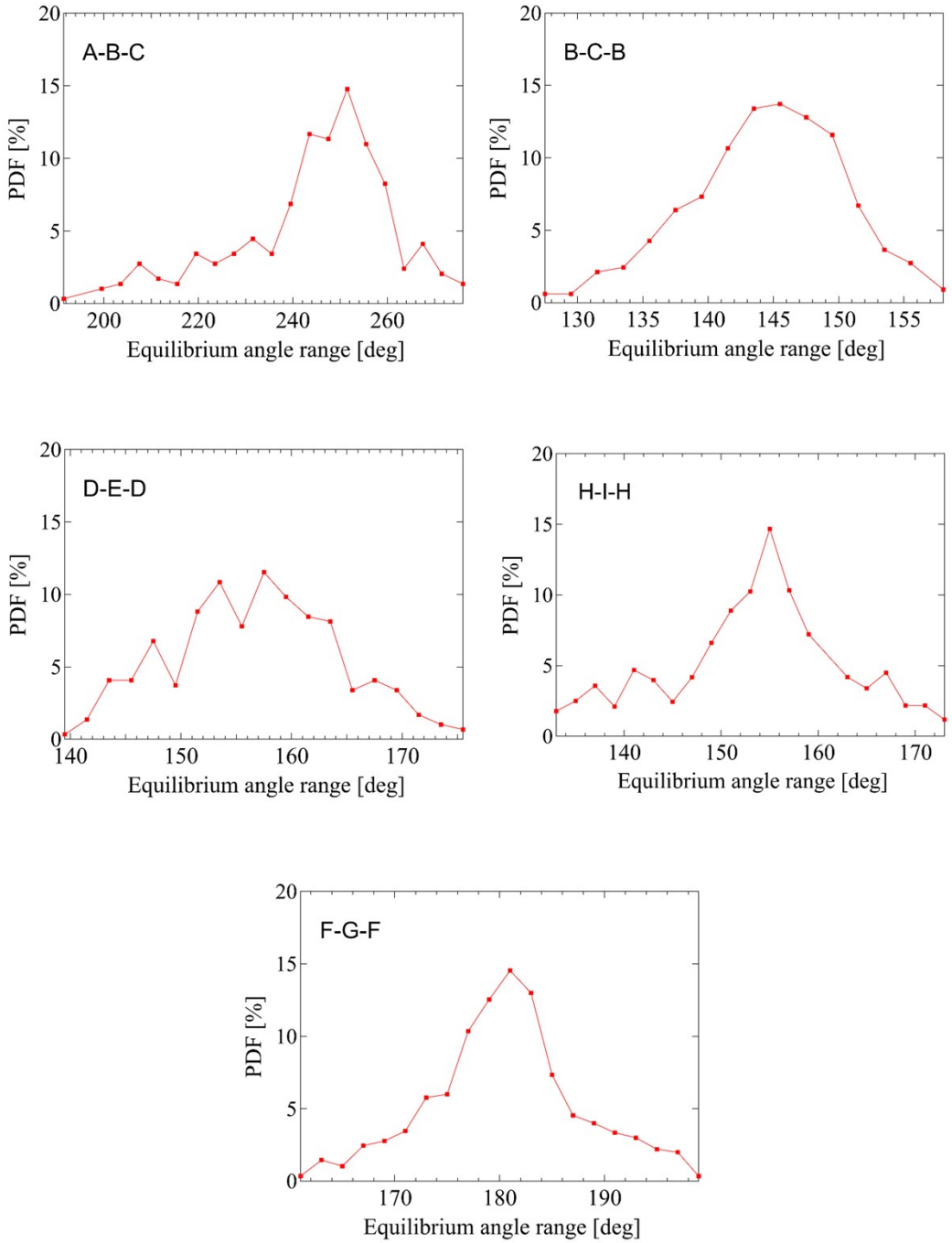

Fig. S3 Equilibrium angle in DGEBA/4,4'-DDS, DGEBA/MPDA and DGEBA/DETA system. DGEBA includes A, B, C beads. 4,4'-DDS includes D, E beads. MPDA includes F, G beads. DETA includes H, I beads.