# SUPPORTING INFORMATION

for

## "Structure of a Thermoset Polymer near an Alumina Substrate as Studied by Dissipative Particle Dynamics"

by

Gokhan Kacar, Elias A. J. F. Peters, and Gijsbertus de With*

*Laboratory of Materials and Interface Chemistry, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, P.O. Box 513, 5600 MB, Eindhoven, The Netherlands.*

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* E-mail: g.dewith@tue.nl, Tel.: +31-40-247-4947

**DPD interaction parameters used in the simulations**

**Table S1.** Liquid mass densities ($\rho_{m,i}$), molecular weights (MW), pure component number densities ($\rho_{i,\text{pure}}$), and solubility parameters ($\delta_i$).

| Type of Bead | $\rho_{m,i}$ ($g/cm^3$) | MW (g/mol) | $\rho_{i,\text{pure}} = \rho_{m,i}/\text{MW}$ ($Å^{-3}$) | $\delta_i$ $((J/cm^3)^{0.5}$) |
|---|---|---|---|---|
| A | 0.938 | 58.07 | 0.0097 | 20.02 |
| B | 1.034 | 94.11 | 0.0066 | 29.08 |
| C | 0.634 | 44.09 | 0.0087 | 16.11 |
| F | 0.987 | 60.09 | 0.0098 | 31.91 |
| D | 1.034 | 31.05 | 0.0200 | 27.74 |
| E | 1.001 | 45.08 | 0.0134 | 21.64 |
| A′ | 0.821 | 46.07 | 0.0107 | 25.09 |
| D′ | 1.001 | 45.08 | 0.0133 | 21.64 |
| D′′ | 0.825 | 59.11 | 0.0084 | 18.07 |
| E′ | 0.825 | 59.11 | 0.0084 | 18.07 |

**Table S2.** The DPD interaction parameters of beads are present in the system before and after cross-linking.

| $a_{ij}/k_BT$ | **A** | **B** | **C** | **F** | **D** | **E** | **A′** | **D′** | **D′′** | **E′** | **Alumina** |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **A** | 27.79 | 49.86 | 33.22 | 45.55 | 23.37 | 20.23 | 28.56 | 20.23 | 32.83 | 32.83 | 6.19 |
| **B** | 49.86 | 62.01 | 63.11 | 41.61 | 19.26 | 36.01 | 39.16 | 36.01 | 59.89 | 59.89 | 13.19 |
| **C** | 33.22 | 63.11 | 35.46 | 60.99 | 36.43 | 26.66 | 38.49 | 26.67 | 37.01 | 37.01 | 82.12 |
| **F** | 45.55 | 41.61 | 60.99 | 26.83 | 15.66 | 35.51 | 30.97 | 35.51 | 54.52 | 54.52 | 8.41 |
| **D** | 23.37 | 19.26 | 36.43 | 15.66 | 5.84 | 17.47 | 12.84 | 17.47 | 29.70 | 29.70 | 8.67 |
| **E** | 20.23 | 36.01 | 26.66 | 35.51 | 17.47 | 14.15 | 19.81 | 14.15 | 24.84 | 24.84 | 9.19 |
| **A′** | 28.56 | 39.16 | 38.49 | 30.97 | 12.84 | 19.81 | 22.65 | 19.81 | 35.32 | 35.32 | 7.01 |
| **D′** | 20.23 | 36.01 | 26.67 | 35.51 | 17.47 | 14.15 | 19.81 | 14.15 | 24.84 | 24.84 | 9.19 |
| **D′′** | 32.83 | 59.89 | 37.01 | 54.52 | 29.70 | 24.84 | 35.32 | 24.84 | 37.74 | 37.74 | 85.01 |
| **E′** | 32.83 | 59.89 | 37.01 | 54.52 | 29.70 | 24.84 | 35.32 | 24.84 | 37.74 | 37.74 | 85.01 |
| **Alumina** | 6.19 | 13.19 | 82.12 | 8.41 | 8.67 | 9.19 | 7.01 | 9.19 | 85.01 | 85.01 | 25.00 |

**Table S3.** Bond potential parameters of the equation: $V_{\mathrm{B},ij}\left(r\right)=k_{ij}\left(r-r_{0,ij}\right)^{2}$ used in the simulations.

| Bond type | $k_{ij}$ $[k_{\mathrm{B}}T/r_{\mathrm{DPD}}{}^{2}]$ | $r_{0,ij}$ $[r_{\mathrm{DPD}}{}^{2}]$ |
|---|---|---|
| A-B | 500.0 | 0.65 |
| B-C | 500.0 | 0.54 |
| D-E | 500.0 | 0.43 |
| A'-D' | 500.0 | 0.44 |
| B-F | 500.0 | 0.63 |
| A'-D'' | 500.0 | 0.44 |
| A'-B | 500.0 | 0.65 |
| D'-E | 500.0 | 0.43 |
| D''-E | 500.0 | 0.43 |
| D-E' | 500.0 | 0.43 |
| D'-E' | 500.0 | 0.43 |
| D''-E' | 500.0 | 0.43 |
| A'-E' | 500.0 | 0.53 |

**Table S4.** Angle potential parameters of the equation: $V_{\mathrm{A},ijk}\left(\theta\right) = k_{ijk}\left(\theta - \theta_{0,ijk}\right)^2$ used in the simulations.

| Angle type | $k_{ijk}$ [$k_\mathrm{B}T$/rad$^2$] | $\theta_{0,ijk}$ [deg] |
|---|---|---|
| A-B-C | 50.0 | 170.6 |
| B-C-B | 50.0 | 94.7 |
| B-F-B | 50.0 | 117.1 |
| C-B-F | 50.0 | 172.3 |
| D-E-D | 50.0 | 163.4 |
| A'-B-C | 50.0 | 170.6 |
| D-E'-D | 50.0 | 163.4 |
| D'-E-D | 50.0 | 163.4 |
| D'-E'-D | 50.0 | 163.4 |
| D''-E-D | 50.0 | 163.4 |
| D''-E'-D | 50.0 | 163.4 |