Supporting Material

Computer Simulation of PEO/Layered-Silicate Nanocomposites: 2. Lithium Dynamics in PEO/Li^+ Montmorillonite Intercalates

V. Kuppa and E. Manias*

Force-field parameters for the MD simulations

Atom type[1,2]	symbol	mass [amu]	q [e]
Hydrogen PEO	HP	1.0078	0.097
Carbon PEO (CH_3)	C3	12.0000	-0.163
Carbon PEO (CH_2)	C2	12.0000	-0.066
Oxygen PEO	OP	15.9949	-0.256
Lithium	LI	6.9410	1.000
Silicon (MMT)	SI	28.0855	1.200
Oxygen (MMT octahedral)	O3	15.9949	-1.717
Oxygen (MMT cleavage)	OZ	15.9949	-0.800
Oxygen (MMT tetrahedral)	OS	15.9949	-1.000
Aluminum (MMT)	AL	26.9820	2.812
Hydrogen (MMT octahedral OH)	HA	1.0078	0.717

PEO force-field parameters[2]		
Non-bonded	$V(r)=C_{12}/r^{12}-C_6/r^6 \quad + q_1q_2/4\pi\epsilon r$	
self	C_6 [KJ/mole nm^6]	C_{12} [KJ/mole nm^{12}]
HP	1.4520e-04	1.12137e-07
C3	2.8150e-03	4.95262e-06
C2	2.8150e-03	4.95262e-06
OP	1.8162e-03	9.75124e-07
cross-terms		
C-OP	2.2262e-03	1.9191e-06
C-HP	5.7948e-04	3.6740e-07
OP-H	4.8212e-04	3.0317e-07
atom pairs		
HP-LI	1.3803e-03	4.0331e-08
C-LI	1.7637e-02	6.5347e-06
OP-LI	1.7888e-03	6.8371e-08

[1] F-R. C. Chang, N. T. Skipper, and G. Sposito, Langmuir. **138**, 2074 (1997)

[2] G.D. Smith, R. L. Jaffe, and D. Y. Yoon, J. Phys. Chem. **97**, 12752 (1993)

PEO bonded parameters[2]		
Bond-Stretching	$V(r)=(k_b/2)\ (r-b_o)^2$	
bond	b_o [nm]	k_b [KJ/mol]
HP - C3	0.10900	273790
HP - C2	0.10900	273790
C2 - C2	0.15100	258324
C3 - OP	0.13900	308902
C2 - OP	0.13900	308902
Bond-Angle	$V(\theta)=(k_\theta/2)\ (\theta_{ijk}-\theta_o)^2$	
angle	θ_o [deg]	k_θ [KJ/(mol rad^2)]
HP - C3 - OP	110.0709	470.40
HP - C2 - OP	110.0709	470.40
HP - C3 - HP	108.3000	323.40
HP - C2 - HP	108.3000	323.40
HP - C2 - C2	109.4870	361.20
C2 - C2 - OP	109.0396	722.40
C3 - OP - C2	111.5606	625.18
C2 - OP - C2	111.5606	625.18
C-O Dihedral	$V_{ijkl}(\phi)=k_\phi\ [1+\cos(n\ \phi - \phi_o)]$ cis at 0° and $\phi \equiv (ijk)\angle(jkl)$	
dihedrals	ϕ_o [deg]	k_ϕ [KJ/mol] n
- C2 - OP -	0.0	5.88 3
- C3 - OP -	0.0	5.88 3
Ryckaert-Bellemans	$V_{ijkl}(\phi)=\sum_{i=0}^{5}\ C_i\ cos^i(\phi)$	
C-C dihedrals	C_0, C_1, C_2, C_3, C_4, C_5 [all in KJ/mol]	
- C2 - C2 -	5.7799, 12.76, 7.3199, -3.2594, -3.760, -16.495	

MMT/PEO amd MMT/Li force-field parameters[3]		
	$V(r)=C_{12}/r^{12}-C_6/r^6$	
atom pairs	C_6 [KJ/mole nm^6]	C_{12} [KJ/mole nm^{12}]
LI - O	2.9297e-02	7.1526e-06
LI - SI	3.7674e-02	3.0328e-05
LI - AL	1.3923e-01	2.6098e-03
LI - HA	7.2458e-05	8.2153e-09
C - O	2.2262e-03	1.9191e-06
C - SI	1.0050e-01	1.6362e-05
C - AL	1.0050e-01	1.6362e-05
C - HA	5.7948e-04	3.6740e-07
OP - O	1.7489e-03	1.3534e-06
OP - SI	5.7734e-03	8.6722e-06
OP - AL	5.7734e-03	8.6722e-06
OP - HA	4.8212e-04	3.0317e-07

Melting Points for the Simulated bulk PEO

Bulk PEO crystal-to-amorphous transition Temperature			
criterion		T_m [K]	error [K]
ttg	melting	353	±20
ttgttg	melting	355	±15
ttgttgttg	melting	352	±15

[3] E. Hackett, E. Manias, and E. P. Giannelis, J. Chem. Phys. **108**, 7410, (1998)