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Coarse-grained molecular dynamics simulations of nanoscale roughness effects on oil film delamination

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Author names and affiliation:

Shizhe Deng, Department of Mechanical Engineering, Graduate School of Engineering, The University of Tokyo, 7-3-1 Hongo Bunkyo-ku, Tokyo, 113-8654, Japan.

Atsushi Kubo, Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba Meguro-ku, Tokyo, 153-8505, Japan.

Yoshikazu Todaka, Department of Mechanical Engineering, Toyohashi University of Technology, 1-1 Hibarigaoka, Tempaku, Toyohashi, 441-8580, Aichi, Japan.

Yoshinori Shiihara, Graduate School of Engineering, Toyota Technological Institute, 2-12-1 Hisakata, Tempaku-ku, Nagoya, 468-8511, Aichi, Japan.

Masatoshi Mitsuhashi, Department of Advanced Materials Science and Engineering, Faculty of Engineering Sciences, Kyushu University, Kasuga-shi, Fukuoka, 816-8580, Japan

Yoshitaka Umeno, Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba Meguro-ku, Tokyo, 153-8505, Japan.

E-mail address of the corresponding author:

umeno@iis.u-tokyo.ac.jp.

Appendix

Modeling method

A hybrid modeling method including united-atom and coarse-grained method is applied in this work. Figure 12 shows the schematic illustration of such hybrid modeling method.

Potential parameters

The parameters of CG force field employed in this study are provided in Tab. 1 and Tab. 2 as following:

Surface distance

Surface distance of all cases are provided in Tab. 3. The temporal evolution of normal stress and shear stress of Case A in Fig. 5 are shown in Fig. 13. The average stresses were calculated from the last 10 ns of total 100 ns.

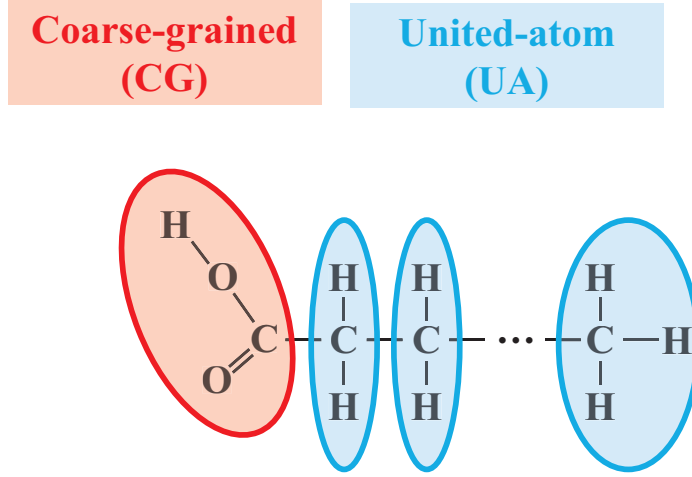


Fig. 12 Schematic Illustration of modeling method used in this work, including both united-atom (blue) and coarse-grained (red) method.

Table 1 Potential function parameters for non-bond interactions [21, 43, 44].

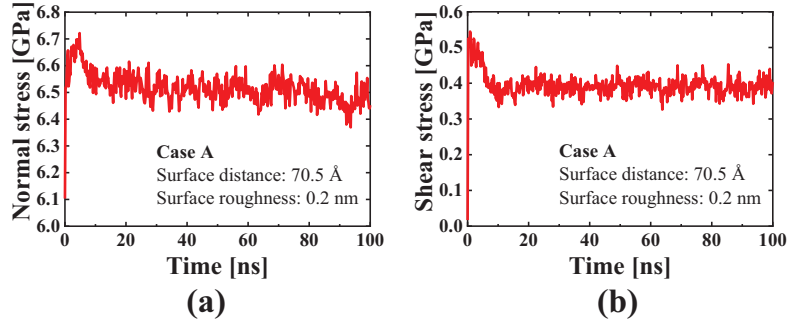
Pair interactions	α [kcal/mol]	β [Å]
CH ₂ -CH ₂	0.1400	3.9650
CH ₂ -COOH	0.2049	4.2118
Fe-CH ₂	0.2499	4.2999
Fe ^{SP} -CH ₂	0.2499	4.2999
COOH-COOH	0.3000	4.4740
Fe-COOH	0.3658	4.5675
Fe ^{SP} -COOH	12.8000	4.5675

Table 2 Potential function parameters for bonding interactions within lubricants [21, 43, 44].

K^b [kcal/mol Å ⁻²]	r_0 [Å]	K^a [kcal/mol]	θ_0 [°]		
115	1.54	60	109		
K_1^d [kcal/mol]	ϕ_1 [°]	K_2^d [kcal/mol]	ϕ_2 [°]	K_3^d [kcal/mol]	ϕ_3 [°]
3.02	180	-0.56	0	2.58	180

Table 3 Surface distance of all cases.

Surface roughness [nm]	0	0.1	0.2	0.3	0.4	0.5
Surface distance [Å]	59	61	69	69	73	77
	61	63	69.5	69.5	75	79
	63	65	70	70	77	81
	65	65.5	70.5	70.5	79	83
	65.5	66	72	71	81	85
	66	66.5	73	71.5	83	87
	66.5	67	75	72	85	89
	67	69	77	72.5	87	91
	69	71	79	73	89	93
	71	73	81	75	91	95
	73	75	83	77	93	97
	75	77	85	79	95	99
	77	79	87	81	97	101

**Fig. 13** Temporal evolution of normal stress and shear stress of Case A in Fig. 5 with the surface distance of 70.5 Å and surface roughness of 0.2 nm.