Supporting Information

Addition of low concentrations of an ionic liquid to a base oil reduces friction over multiple length scales: a combined nano- and macrotribology investigation

Hua Li,^a Anthony E. Somers,^b Patrick C. Howlett,^b Mark W. Rutland,^c Maria Forsyth,^b and Rob Atkin^{a,*}

^{*a*} Priority Research Centre for Advanced Fluids and Interfaces, The University of Newcastle, Callaghan, NSW 2308, Australia

^b Institute for Frontier Materials, Deakin University, 221 Burwood Highway, Burwood, Victoria 3125, Australia

^c School of Chemical Science and Engineering, KTH Royal Institute of Technology, SE100 44 Sweden, and Chemistry, Materials and Surfaces, SP Technical Research Institute of Sweden

E-mail: rob.atkin@newcastle.edu.au

Calculation of Herzian contact stress

The effective Young's modulus E_w can be calculated by

$$\frac{1}{E_w} = \frac{1}{2} \left(\frac{1 - v_1^2}{E_1} + \frac{1 - v_2^2}{E_2} \right)_{,(1)}$$

where E_1, E_2 are the elastic moduli and v_1, v_2 the Poisson's ratios associated with each body

Contact area of radius
$$a \approx (\frac{3RF}{2E_w})^{1/3}$$
, (2)

where R is the sphere radius, F is applied load

Contact stress:
$$p_{max} = \frac{3F}{2\pi a^2}$$
 (3)

The parameters used: Silica: E=73 GPa v=0.17; silicon: E=165 GPa, v=0.27; Silicon nitride: E=231.5 v=0.25

Therefore, in the nanotribology tests

$$F=160 \text{ nN}, p_{max} \approx 1.2 \text{ GPa}$$
$$F=300 \text{ nN}, p_{max} \approx 2.1 \text{ GPa}$$

Macrotribology test

$$F=2N, p_{max} \approx 1.2 GPa$$
$$F=10N, p_{max} \approx 2.1 GPa$$

Hamrock and Dowson model

This model is based on the Hertz model of contact stresses. It is discussed in detail in Stachowiak's book *Engineering Tribology*.¹ In this model, the central film thickness, h_c , can be calculated in the following equation:

$$\frac{h_c}{a} = 2.69 \left(\frac{V\eta_0}{E_w a}\right)^{0.67} (\alpha E_w)^{0.53} \left(\frac{F}{E_w a^2}\right)^{-0.067} (1 - 0.61e^{-0.73k})$$
(4)

where *a* is the contact area radius from eq(2), *V* is sliding velocity, η_0 is the viscosity of the lubricant at ambient pressure, E_w is the effective Young's modulus from eq(1),*a* is the pressure-viscosity coefficient, *F* is the applied load, and *k* is the ellipticity parameter. *k*=1 for point contact. The pressure-viscosity coefficient of hexadecane varies from 11.6 to 13.2, an average of 12.5 is used here.² For the pure IL used in this study, the pressure-viscosity coefficient was not found in the literature. According to previous studies, the pressure-viscosity coefficient of ILs are generally between 12~21 GPa⁻¹, ³⁻⁶ thus here the film thicknesses of the systems are calculated by assuming the limit values of 12 GPa⁻¹ and 21 GPa⁻¹ for the pure IL and the pressure-viscosity coefficients of the mixtures are calculated by molar ratio, as shown in Table S1 and Table S2.

The table below show the calculated film thicknesses do not vary significantly for different chosen values of the pressure-viscosity coefficient, especially for the IL-hexadecane mixtures.

Table S1. The pressure-viscosity coefficients and calculated film thickness when assuming the pressure-viscosity coefficient (α) of pure IL is 12.

		hexadecane	0.01 mol% IL	1.0 mol% IL	10 mol% IL	Pure IL
α		12.5	12.5	12.5	12.4	12.0
Calculated Film	2 N	2.6	2.7	2.8	4.0	118
thickness (nm)	10 N	2.4	2.5	2.6	3.5	106

		0.01 mol% IL	1.0 mol%	10 mol% IL	Pure IL
			IL		
α		12.5	12.6	13.4	21.0
Calculated Film	2 N	2.7	2.8	4.1	159
thickness (nm)	10 N	2.5	2.6	3.7	143

Table S2. The pressure-viscosity coefficients and calculated film thickness when assuming the pressure-viscosity coefficient (α) of pure IL is 21.

Table S3. Zero shear viscosity of IL-hexadecane mixtures at 20 °C measured by an AR-G2 rheometer (TA instruments).

IL concentration	hexadecane	0.01 mol%	1 mol%	10 mol%	Pure IL
Viscosity (mPa s)	3.8	3.9	4.0	6.7	1007
Density (g/cm ³)	0.773 ⁷	0.773ª	0.776ª	0.802 ^a	0.885 ⁸
			. .		

^aThe values are calculated from the weight concentration of the IL and the hexadecane in the mixture.

- 1. G. W. Stachowiak and A. W. Batchelor, *Engineering Tribology*, Butterworth-Heinemann, 2001.
- 2. M. Hartl, I. Krupka, R. Poliscuk, M. Liska, J. Molimard, M. Querry and P. Vergne, *Tribol. Trans.*, 2001, 44, 270-276.
- 3. X. Paredes, O. Fandiño, A. S. Pensado, M. J. P. Comuñas and J. Fernández, *Tribol Lett*, 2012, 45, 89-100.
- 4. A. S. Pensado, M. J. P. Comuñas and J. Fernández, *Tribol Lett*, 2008, 31, 107-118.
- 5. F. M. Gaciño, M. J. P. Comuñas, T. Regueira, J. J. Segovia and J. Fernández, *The Journal of Chemical Thermodynamics*, 2015, 87, 43-51.
- 6. G. Mordukhovich, J. Qu, J. Y. Howe, S. Bair, B. Yu, H. Luo, D. J. Smolenski, P. J. Blau, B. G. Bunting and S. Dai, *Wear*, 2013, 301, 740-746.
- 7. M. S. D. S. Hexadecane, Sigma-Aldrich.
- 8. C. M. S. S. Neves, P. J. Carvalho, M. G. Freire and J. A. P. Coutinho, *The Journal of Chemical Thermodynamics*, 2011, 43, 948-957.