Supplementary Material

Kinetics Study of the Al-Water Reaction Promoted by an Ultrasonically Prepared

Al(OH)₃ Suspension

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1. The maximum contact area between two spheres during colliding

If two elastic spheres with the mass, radius and velocity of m_1 , r_1 , v_1 and m_2 , r_2 , v_2 , respectively, collide along one line, as shown in Fig. S1, there will be a deformation zone around the colliding point for each sphere. When the two spheres' velocities

reach the same value (v) during colliding, their contact area is maximum. According to the momentum conservation law

$$m_1 v_1 + m_2 v_2 = (m_1 + m_2) v \tag{S1}$$

we can obtain

$$v = \frac{m_1 v_1 + m_2 v_2}{m_1 + m_2} \quad . \tag{S2}$$

If the collision is elastic, the total deformation potential energy of two spheres at the moment is

$$\Delta E = \frac{1}{2} m v_1^2 + \frac{1}{2} m v_2^2 - \frac{(m_1 v_1 + m_2 v_2)^2}{2(m_1 + m_2)}$$

= $\frac{1}{2} \frac{m_1 m_2}{m_1 + m_2} (v_1 - v_2)^2$
= $\frac{1}{2} \mu (v_1 - v_2)^2$ (S3)

where μ is the reduced mass.

If the deformation of the sphere is elastic, there is the following relation between the stress (σ) and strain (ε)

$$\sigma = E\varepsilon \tag{S4}$$

where *E* is the Young's modulus. Because the gravity center of a sphere is at its center, as an approximation, the strains of two spheres during colliding can be written

$$\varepsilon_1 = \frac{x_1}{r_1}$$

$$\varepsilon_2 = \frac{x_2}{r_2}$$
(S5)

where x_1 and x_2 are the deformations of sphere 1 and sphere 2 during colliding, respectively. According to the Newton's third law, the acting force is equal to the reacting force

$$F_1 = F_2$$

$$E_1 \varepsilon_1 S_1 = E_2 \varepsilon_2 S_2$$
(S6)

where S_1 and S_2 are the deformation areas of sphere 1 and sphere 2 during colliding, respectively. If the materials of two spheres have the same Young's modulus (*E*), then

$$E\varepsilon_{1}S_{1} = E\varepsilon_{2}S_{2}$$

$$E\varepsilon_{1}\pi R_{1}^{2} = E\varepsilon_{2}\pi R_{2}^{2}$$

$$\frac{x_{1}}{r_{1}}\pi [r_{1}^{2} - (r_{1} - x_{1})^{2}] = \frac{x_{2}}{r_{2}}\pi [r_{2}^{2} - (r_{2} - x_{2})^{2}] \quad .$$

$$\frac{x_{1}}{r_{1}} [2r_{1}x_{1} - x_{1}^{2}] = \frac{x_{2}}{r_{2}} [2r_{2}x_{2} - x_{2}^{2}]$$
(S7)

As x_1 and x_2 are the small quantities and their quadratic terms can be negligible, then equation (S7) can be written

$$\frac{x_1}{r_1} [2r_1 x_1] = \frac{x_2}{r_2} [2r_2 x_2]$$

$$x_1^2 = x_2^2$$
(S8)

finally we get

$$x_1 = x_2 \quad . \tag{S9}$$

The deformation potential energies of two spheres can be calculated

$$w_{1} = \int_{0}^{x_{1}} F_{1} dx$$

$$= \int_{0}^{x_{1}} E \frac{x_{1}}{r_{1}} \pi [r_{1}^{2} - (r_{1} - x_{1})^{2}] dx$$

$$= \int_{0}^{x_{1}} E \frac{\pi}{r_{1}} [2r_{1}x_{1}^{2} - x_{1}^{3}] dx$$

$$= \frac{E\pi}{r_{1}} [\frac{2}{3}r_{1}x_{1}^{3} - \frac{1}{4}x_{1}^{4}]$$

$$w_{2} = \frac{E\pi}{r_{2}} [\frac{2}{3}r_{2}x_{2}^{3} - \frac{1}{4}x_{2}^{4}] \quad . \tag{S10b}$$

Neglecting the biquadratic terms of x_1 and x_2 , equation (S10) is simplified as

$$w_1 = \frac{2}{3}\pi E x_1^3$$
(S11a)

$$w_2 = \frac{2}{3}\pi E x_2^3 . (S11b)$$

The total deformation potential energy of two spheres in equation (S3) can be written

$$\Delta E = w_1 + w_2 = \frac{1}{2} \mu (v_1 - v_2)^2$$

$$\frac{2}{3} \pi E x_1^3 + \frac{2}{3} \pi E x_2^3 = \frac{1}{2} \mu (v_1 - v_2)^2$$
(S12)

Using the result in equation (S9), the above equation can be written

$$\frac{4}{3}\pi E x_2^3 = \frac{1}{2}\mu(v_1 - v_2)^2.$$
(S13)

The contact area between two colliding spheres should be the deformation area of the smaller sphere $(r_1 > r_2)$

$$S_{2} = \pi R_{2}^{2}$$

$$= \pi [r_{2}^{2} - (r_{2} - x_{2})^{2}]$$

$$= \pi [2r_{2}x_{2} - x_{2}^{2}]$$

$$\approx 2\pi r_{2}x_{2}$$
(S14)

then

$$x_2 = \frac{S_2}{2\pi r_2}.$$
 (S15)

Inserting the above result into equation (S13), we obtain

$$\frac{ES_2^3}{6\pi^2 r_2^3} = \frac{1}{2} \mu (v_1 - v_2)^2.$$
(S16)

Then

$$S_{2} = r_{2} \sqrt[3]{\frac{3\pi^{2}\mu}{E} (v_{1} - v_{2})^{2}}$$

= $r_{2} \sqrt[3]{\frac{3\pi^{2}\mu}{E} v_{12}^{2}}$ (S17)

The relative average speed of two spheres with the Maxwell-Boltzmann rate distribution can be obtained by vector calculation [1] (please see the text)

$$\bar{v_{12}} = \sqrt{\frac{8kT}{\pi\mu}} \quad . \tag{S18}$$

As the statistical average, the maximum contact area between two spheres (Brownian particles) during colliding can be obtained

$$S = 2r_2 \sqrt[3]{\frac{3\pi kT}{E}} \quad . \tag{S19}$$

Reference

[1] Qin YH. Thermodynamics, Higher Education Press, Beijing, 2008.



Fig. S1. Schematic representation of the elastic collision between two spheres with different momentums and their deformation $(r_1 > r_2)$.