van der Waals Potentials

Approximate van der Waals interactions with arbitrary shapes can be found by integrating the contribution from each volume element:

$$dU = -\frac{\beta}{\rho^6}\cdot dV$$

The most fundamental geometry is that of a half space where the potential above the surface by a distance h is

$$U(h) = \int_h^\infty \int_0^\infty \frac{-\beta}{\left(z^2 + r^2\right)^3}\cdot 2\cdot\pi\cdot r\,dr\,dz \qquad \text{or} \qquad U(h) = -\frac{\beta\cdot\pi}{6\cdot h^3}$$

Redefining the potentials in terms of the half space form gives

$$U(h) = -\frac{\alpha}{h^3} \qquad \text{and originally,} \qquad dU = -\frac{6\cdot\alpha}{\pi\cdot\rho^6}\cdot dV$$

For the surface of a sphere radius a, with h the distance from the surface,

$$U(h) = -\frac{8\cdot\alpha\cdot a^3}{h^3\cdot(h + 2\cdot a)^3} \qquad a < 0 \ \text{works for a hollow cavity}$$

A one dimensional arbitrary corregation with attractive material filling the space z<f(x) has the potential

$$U(x,z) = -\frac{\alpha}{z^3} - \frac{3\cdot\alpha}{4}\cdot\int_{-\infty}^{\infty} \frac{1}{(x-u)^4}\cdot(Q(z) - Q(z - f(u)))\,du \qquad Q(t) = t\cdot\frac{3\cdot(x-u)^2 + 2\cdot t^2}{\left[(x-u)^2 + t^2\right]^{\frac{3}{2}}}$$

convenient for numenrical integration. Care must be taken through the region near x=u.

For practical reasons, it is convenient to define a van der Waals strength in terms of a temperature, T_v, representing the approximate single particle binding energy to the flat surface, in this case gold.

$$k := 1.38\cdot 10^{-23} \qquad T_v := 39 \qquad m_4 := 6.6\cdot 10^{-27} \qquad z_1 := 3.578\cdot 10^{-10} \qquad \text{(MKS units)}$$

$$U(z) := -\frac{k\cdot T_v}{m_4}\cdot\left(\frac{z_1}{z}\right)^3 \qquad \text{(energy per unit mass)}$$

The helium mass is m_4, the monolayer thickness is z_1, and k is Boltzman's constant. One final refinement accounts for retardation effects at far distances, where the potential crosses over to a $1/z^4$ form. The factor of $z_r = 41.7 \cdot z_1$ is traditional for glass and may not be appropriate for gold.

$$z_r := 41.7 \cdot z_1 \qquad U(z) := -\frac{k \cdot T_v}{m_4} \cdot \left(\frac{z_1}{z}\right)^3 \cdot \frac{1}{1 + \frac{z}{z_r}}$$