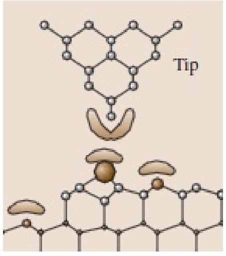
STUDY :

Introduction : Results are matched with H-H atoms moleculer forces and a typical Si-Si interaction graphics from Bushan's Springer Link Hand Book of Nano Technology



H-H vals:
b = 2.5e10; % decay factor
a = 74*PM; % bond distance 2.42 A in m
D = 436; % Bond Energy per kj/mol

Si-Si vals:
a = 296*PM; % bond distance 2.42 A in m
D = 130; % Bond Energy per kj/mol
b = 2.5e10; % decay factor

$$V_{\mathrm{vdW}} = -\frac{A_{\mathrm{H}}}{6z} . \tag{13.1}$$

The "Hamaker constant", A_{H}, depends on the type of materials (atomic polarizability and density) of the tip and sample and is on the order of 1 eV for most solids [13.13].

When the tip and sample are both conductive and have an electrostatic potential difference, $U \neq 0$, electrostatic forces are important. For a spherical tip with radius R, the force is given by [13.14]:

$$F_{\mathrm{electrostatic}} = -\frac{\pi \varepsilon_0 R U^2}{z} . \tag{13.2}$$

Chemical forces are more complicated. Empirical model potentials for chemical bonds are the Morse potential (see e.g., [13.13]).

$$V_{\mathrm{Morse}} = -E_{\mathrm{bond}} \left(2\mathrm{e}^{-\kappa(z-\sigma)} - \mathrm{e}^{-2\kappa(z-\sigma)} \right) \tag{13.3}$$

and the Lennard-Jones potential [13.13]:

$$V_{\mathrm{Lennard\text{-}Jones}} = -E_{\mathrm{bond}} \left(2\frac{\sigma^6}{z^6} - \frac{\sigma^{12}}{z^{12}} \right) . \tag{13.4}$$

These potentials describe a chemical bond with bonding energy E_{bond} and equilibrium distance σ. The Morse potential has an additional parameter – a decay length κ.

The Hamaker constant

The Hamaker constant consists of the prefactor to the van der Waal's integral.

$$A = \left(\frac{\rho N_A}{M} \right)^2 \pi^2 \beta$$

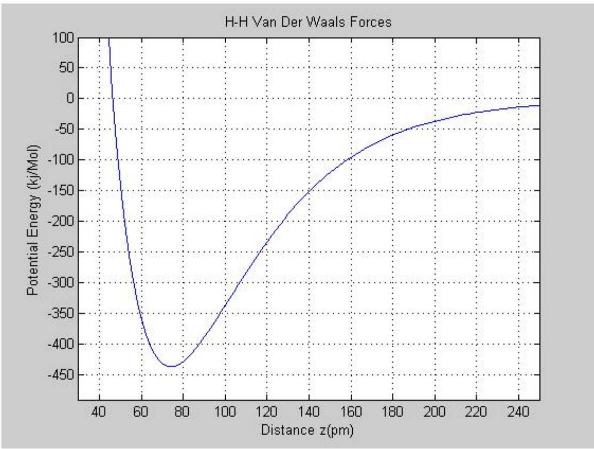
The order of magnitude of the Hamaker constant can be estimated based on the following considerations. For cases where the dispersion interaction is the dominant contribution.

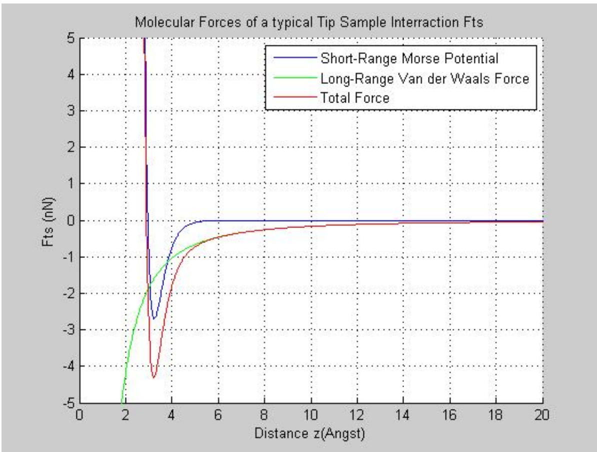
$$\beta = \frac{3}{4} h\nu \left(\frac{\alpha}{4\pi\varepsilon_0} \right)^2$$

Recognize that $\rho N_A/M$ is the reciprocal of the molecular volume and $\alpha/4\pi\varepsilon_0$ is about 10% of the atomic volume. Therefore $A \approx 3/4\pi^2 h\nu(0.1)^2 \approx 10^{-18}$ J.

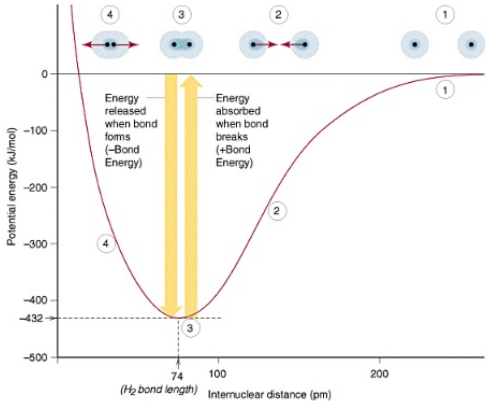
```
clear all;
close all;
clc

% kc=42; % cantilever stiffness
% wc = 300*10^3*2*pi; % cantilever natural frequency
% mc = kc/wc^2 ; % cantilver mass
% LinPot=2*D*b^2; % Potential is Linearized from Akays Paper

Angst=1e-10;                 % Angstrom;
Nano=1e-9;                   % Nano Scale Factor
PM=Angst/100;                % PicoMeter
Avagadro=6.022142*10^23;     % Avagadro number
AH=1e-18;                      % Hamaker constant in eV;
kN2N=1e3;                    % Kilo Newton to Newton

b = 2.5e10;          % decay factor
a = 74*PM;           % bond distance 2.42 A in m
D = 436;             % Bond Energy per kj/mol

z=linspace(0,20*Angst,1000);
z=z';

VMorse=-D*(2*exp(-b*(z - a))-exp(-2*b*(z - a))); % kJ/mol
FMorse=(2*b*exp(b*(a - z)) - 2*b*exp(2*b*(a - z)))*D; % kNewton /mol

FMorsePerMolecule=FMorse/Avagadro*kN2N; % Newton per molecule

% Decay Factor Confirmation From a Web Source using H-H Bond
% http://www.science.uwaterloo.ca/~cchieh/cact/c120/bondel.html

plot(z/PM,VMorse);
set(gca,'XLim',[30 250]);
set(gca,'YLim',[-490 100]);
grid;

title('H-H Van Der Waals Forces');
xlabel('Distance z(pm)')
ylabel('Potential Energy (kj/Mol)');


% AFM Moleculer Force Confirmation : Bushan Springers HandB. of Nano.
clear VMorse FMorse FMorsePerMolecule;

a = 296*PM;           % bond distance 2.42 A in m
D = 130;             % Bond Energy per kj/mol
b = 2.5e10;          % decay factor

VvdW=-AH./(6*z);
FvdW=AH./(6.*z.^2);

VMorse=-D*(2*exp(-b*(z - a))-exp(-2*b*(z - a))); % kJ/mol
FMorse=(2*b*exp(b*(a - z)) - 2*b*exp(2*b*(a - z)))*D; % kNewton /mol
FMorsePerMolecule=FMorse/Avagadro*kN2N; % Newton per molecule

FTotal=FMorsePerMolecule/Nano+FvdW;

figure;
hold;

plot(z/Angst,-FMorsePerMolecule/Nano,'-b');
plot(z/Angst,-FvdW,'-g');
plot(z/Angst,-FTotal,'-r');

set(gca,'XLim',[0 20]);
set(gca,'YLim',[-5 5]);
grid;
title('Molecular Forces of a typical Tip Sample Interraction Fts');
xlabel('Distance z(Angst)');
ylabel('Fts (nN)');

legend('Short-Range Morse Potential', 'Long-Range Van der Waals Force','Total Force');
```

Results:





Results of Literature:



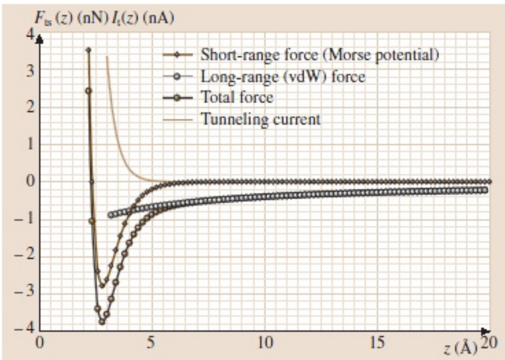


Fig. 13.4 Plot of tunneling current I_t and force F_{ts} (typical values) as a function of distance z between front atom and surface atom layer

Conclusion:

Key Findings - Notes: