Gas-Surface Interaction

- If we want to solve the Boltzmann equation, we need to specify boundary conditions for the velocity distribution function at solid surfaces. Thus, we need to know how incident molecules interact with a solid surface.

- In other words, we need to have a model of *gas-surface interaction*.

- In general, molecules can be adsorbed, move around the surface or undergo chemical reaction with the surface molecules. We will treat collisions as instantaneous and local.

- Accurate modeling of gas surface interaction is very complicated due to lack of complete knowledge of surface properties (surface finish, cleanliness, adsorbed gas layers, etc.) and due to lack of accurate surface interaction potentials.
Specular Reflection

- **Specular reflection** is mirror-like reflection. Specular reflection happens for
  - Smooth metal surface that has been outgassed through exposure to high vacuum and temperatures (baked surface)
  - The ratio of molecular weights of the gas to that of the surface molecules is small in comparison to unity
  - The translational energy of molecules relative to the surface is larger than several electron volts

\[ 1 \text{ eV} = 1.6 \times 10^{-19} \text{ J} \]

Thus, for \( N_2 \) (m=4.65\times10^{-26} \text{ kg}) \[ V > 3.7 \text{ km/s} \]
Specular Reflection

- Fluxes for specularly reflected molecules:

\[ N = N_i + N_r = 0 \quad \text{– No net molecular (impermeability condition)} \]

\[ p_r = p_i \text{ or } p = 2p_i \quad \text{– Net normal momentum flux} \]

\[ \tau_r = -\tau_i \quad \tau \quad \text{– No net shear} \]

\[ q_{i, tr} = -q_{r, tr} \text{ or } q = 0 \quad \text{– No net translational energy flux} \]
Diffuse Reflection

- Velocity of reflected molecule is independent of incident velocity. Reflected molecules have a half-range Maxwellian distribution corresponding to the wall temperature and velocity.

- Fully accommodated diffuse reflections are typical for microscopically rough surfaces and low-speed flows at common temperatures.

\[
f_r(\vec{v}) = \frac{\beta_w}{\pi^{3/2}} e^{-\beta_w \vec{v}^2}, \quad \text{for } (\vec{v}, \vec{n}) > 0
\]

where

\[
\beta_w = \frac{1}{\sqrt{2 R T_w}} \quad \text{and } \vec{n} \text{ is the outward normal to surface.}
\]
Diffuse Reflection (cont)

- Let's calculate fluxes for diffuse reflection.
- Impermeability condition gives $N_r = -N_i$. The reflected molecule flux is then (Bird Eq. (4.22) for stationary gas)

$$N_r = -\frac{n_w}{4} \sqrt{\frac{8}{\pi} R T_w}$$

- Thus,

$$n_w = n_\infty \sqrt{\frac{T_\infty}{T_w}} \left( e^{-s^2 \cos^2 \theta} + \sqrt{\pi} s \cos \theta \right)$$
Diffuse Reflection (cont)

- Normal momentum flux for reflected molecules is (Bird's Eq. (4.25) for stationary gas):

\[ p_r = \frac{n_w m R T_w}{2} = \frac{\rho_w R T_w}{2} = \frac{p_w}{2}. \]

- Parallel momentum flux for reflected molecules is zero (Bird's Eq. (4.26) for stationary gas):

\[ \tau_r = 0. \]
Maxwell suggested a simplified model using two types of interactions that bound the problem: specular and diffuse.

A parameter $\sigma$ is defined to represent the fraction of diffuse reflections and $(1-\sigma)$ is the fraction of specular reflections. The parameter is called [tangential momentum] accommodation coefficient.