

Total ESD rate is a function of several variables

$$R = j_e \cdot \sigma \cdot S \cdot D$$

j_e = incident electron current

σ = excitation cross-section

S = “separation” or desorption probability

D = escape probability

← “Initial state” effects

} “Final state” effects

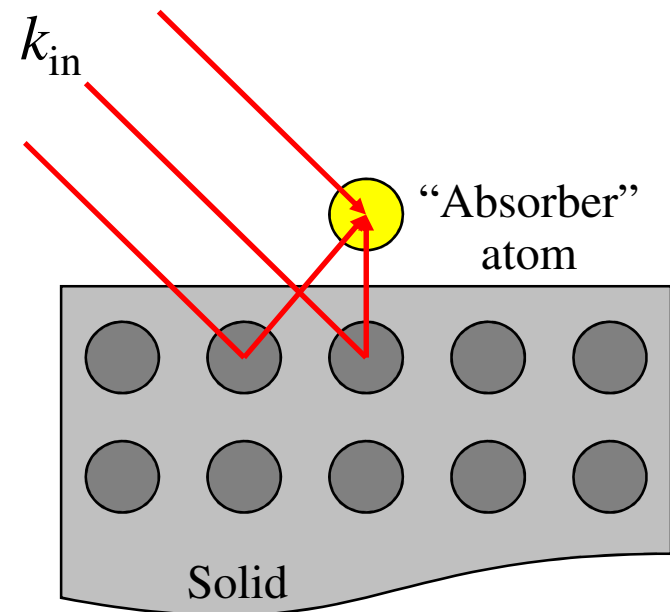
There has been a tremendous amount of work in the past on final-state effects in ESD (velocity distributions, quantum state distributions, ESDIAD, desorption and escape probabilities, etc).

How does scattering and diffraction of the incident electron affect σ ?

Electron scattering, interference, and ESD rates

The incident electron is not really a plane wave, but is the phased sum of a plane wave and all possible scattered waves.

- If the interference is constructive, the electron density at the absorber is high, and the excitation rate is high.
- If the interference is destructive, the electron density at the absorber is low, and the excitation rate is low.
- Whether the interference is constructive or destructive depends upon several factors:
 - ◆ The incident electron energy E .
 - ◆ The incident electron direction relative to the crystal axes.
 - ◆ The local bonding geometry of the absorber atom.



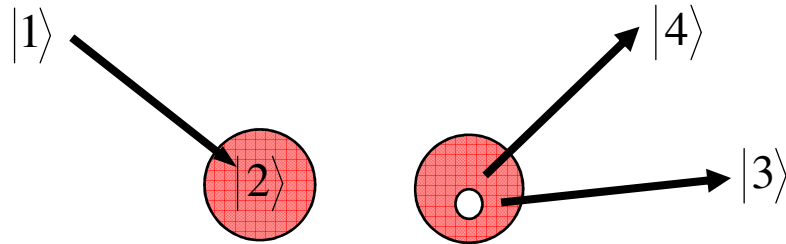
So the ESD rate should depend upon the \mathbf{k} -vector of the incident wave, in a manner unique to the bonding geometry.

The physics is the same as LEED, but the detector is *on the surface*.

Theory

We start with a description of a one-electron excitation by Fermi's Golden Rule:

$$\Gamma_{i \rightarrow f} = 2\pi |\langle 34 | H_{ee} | 12 \rangle|^2 \rho_{if} \delta(E_f - E_i)$$



If we ignore exchange and final-state details, we can write an intuitive expression:

$$\Gamma_{i \rightarrow f} \approx \iint \rho_1(\mathbf{k}, \mathbf{x}) \frac{e^{-a|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|^2} \rho_2(\mathbf{x}') d\mathbf{x} d\mathbf{x}'$$

- Excitation rate is a maximum when the (screened) incident and target electron densities strongly overlap.

In the limit that ρ_2 is strongly localized (core states) and strong screening,

$$\Gamma_{i \rightarrow f} \propto \rho_1(\mathbf{k}, \mathbf{R}_a)$$

$$\rho_1(\mathbf{k}, \mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r})^* \phi_{\mathbf{k}}(\mathbf{r})$$

Method of calculating the initial state

I used a real-space multiple-scattering formalism: Good for localized interactions

In the region between muffin-tin spheres,
the incident electron wave function is given by the Lippman-Schwinger equation:

$$\phi(\mathbf{k}, \mathbf{r}) = \phi_0(\mathbf{k}, \mathbf{r}) + \langle \mathbf{r} | G_0 T | \mathbf{k} \rangle, \quad r > R_{MT}$$

Within the muffin-tin, the
wave function must include
the interaction with the
absorber potential:

$$\phi(\mathbf{k}, \mathbf{r}) = \phi_a(\mathbf{k}, \mathbf{r}) + \int \phi_a(\mathbf{k}', \mathbf{r}) \langle \mathbf{k}' | G_0 t_N (1 + G_0 T) | \mathbf{k} \rangle d\mathbf{k}', \quad r < R_{MT}$$

Zeroth order: Neglect absorber potential and
calculate single-scattering ...

$$\phi_{\mathbf{k}}(\mathbf{R}_a) = \langle \mathbf{R}_a | \mathbf{k} \rangle + \langle \mathbf{R}_a | G_0 t_N | \mathbf{k} \rangle$$

Use atomic scattering t -matrices and special separable curved-wave representation of the free-space propagator G_0 developed by Rehr et al. (PRB **41**, 8139 (1990)).

The real-space method is not entirely satisfactory, because the coulomb interaction demands that we know the incident wave function *everywhere*.

Lots of room for new work here