

# Standing-Wave Electron-Stimulated Desorption (SW-ESD)

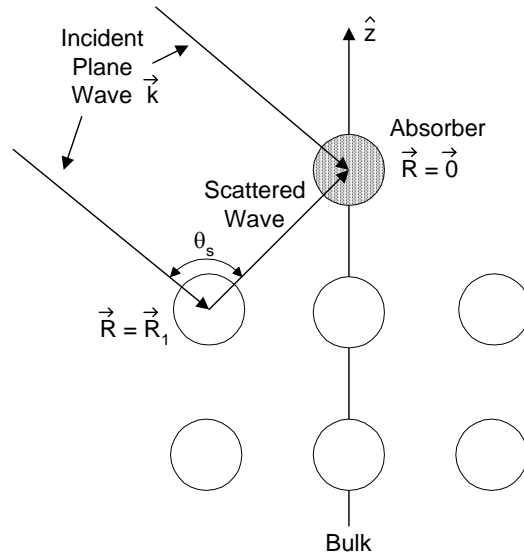
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The total ESD desorption rate can be written as

$$R \propto I(\mathbf{k})\sigma(E)D(E),$$

where  $I(\mathbf{k})$  is the incident electron flux with wavevector  $\mathbf{k}$ ,  $\sigma(E)$  is the cross section for excitation, and  $D(E)$  is the desorption probability. The cross section  $\sigma(E)$  and the desorption probability  $D(E)$  are nominally functions of energy only.  $I$  has been almost universally assumed to be a constant, independent of  $\mathbf{k}$  with respect to the crystal symmetry axes. I show here that this assumption is not necessarily valid, and that it is possible to observe the effect of a varying incident  $\mathbf{k}$ -vector on the desorption rate.

The dependence of the desorption rate on electron  $\mathbf{k}$ -vector is clear if we consider the probability for an electron to impact an atom on a surface.



If we define  $\psi(\mathbf{R} = \mathbf{0})$  to be the electron wave function at the absorber, we must express it as the phased sum of the amplitude to arrive directly at the absorber (the *direct* wave) +

the amplitude to scatter from nearby atoms before arriving at the absorber (the *scattered* waves):

$$\psi(0) = \psi^0 + \psi^1 + \dots + \psi^N,$$

where the superscript denotes the number of scattering events.  $\psi^0$  is simply the value of the plane wave at  $\mathbf{R}=\mathbf{0}$ , and has a constant amplitude and phase which we can arbitrarily choose so that  $\psi^0=1$ :

$$\psi^0 = e^{i\mathbf{k}\cdot\mathbf{R}_0} = 1.$$

In treatments of ESD only this term is retained: higher order scattering terms are neglected. However, it is well-known that the strength of scattering in solids is quite strong, and is the basis for such well-established experimental techniques as LEED and photoelectron diffraction (PED). The singly-scattered wave can be expressed using the amplitude for plane-wave scattering from a free atom:

$$\psi^1 = \sum_{\mathbf{R}_i} e^{i\mathbf{k}\cdot\mathbf{R}_i} f(k, \theta_s) \frac{e^{ikR_i}}{kR_i},$$

where  $f(k, \theta_s)$  is the atomic scattering amplitude, and can be calculated in terms of the partial-wave scattering phase shifts

$$f(\theta) = \sum_{\ell} (2\ell + 1) e^{i\delta_{\ell}} \sin(\delta_{\ell}) P_{\ell}(\cos(\theta)).$$

In general, the phase shifts  $\delta_{\ell}$  are functions of the electron wavenumber  $k$ . The scattering angle  $\theta_s$  is the angle between  $\mathbf{k}$  and  $\mathbf{R}_i$ .

Since the total electron flux at the absorber is given by

$$Flux \propto \psi^*(\mathbf{R} = \mathbf{0}) \psi(\mathbf{R} = \mathbf{0}),$$

it is clear that the flux depends upon the particulars of the scattering, and should depend sensitively upon the incident electron energy and direction. Most importantly, *the total incident flux  $I(\mathbf{k})$  has the symmetry of the absorber bonding site*. The total desorption

yield, then, should carry information about the bonding geometry of the desorbate *before excitation* - this is an important distinction from ESDIAD, which measures the desorption trajectories of the *excited* species, which may not necessarily reflect the true ground state bonding properties.