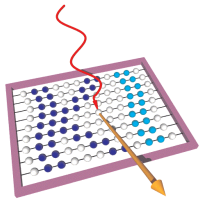

Determination of the Optical Potential for Electron Scattering at Very Low Energies

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Wave Functions of Scattering States

Electron spectroscopy at low kinetic energies, e.g. valence band photoemission with vacuum ultraviolet light, is sensitive to the fine structure of the electron damping, i.e. to the magnitude and energy dependence of the optical potential. The basis of this quantity is usually given by a semiquantitative analytical derivation together with empirical findings from the escape depth.

Only recently the optical potential has been determined ab-initio via calculating the self-energy. Here, this approach is used to calculate the self-energy and from this the wavefunctions in the conduction band regime with scattering boundary conditions for the surface system. For the former, the GW approximation is applied. For the latter, algebraic solvers in the Laue representation have been used to solve the Schrödinger equation for arbitrary potentials. The wavefunction is investigated to extract physical quantities like the angle and energy dependent escape depth, which are significant in discussing electron scattering.

Generally the form of the self-energy will be a function of momentum transfer (non-locality), of frequency (dynamics), and of two reciprocal lattice vectors (local fields). The latter reflect the discrete translational symmetry of the lattice. This dependence is expected not to be far from diagonal behavior with weak variation of the diagonal elements on momentum.

A local LDA-like version of Σ simplifies the calculation and yields characteristic deviations from the homogenous case.

The computation of Σ in the GW approximation:

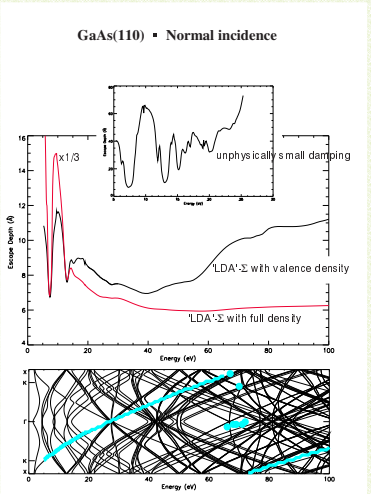
$$\Sigma_{G_1,G_2}(\mathbf{k},\omega) = \frac{ie^2}{(2\pi)^4 v_K}\int d\mathbf{k}' \sum_{G'} \frac{1}{|\mathbf{k}-\mathbf{k}'+\mathbf{G}_1-\mathbf{G}'|^2+\kappa_{TF}^2} \int d\omega' e^{i\omega'\tau} \tau^{-1}(\omega')(G_{G'G'+G_2-G_1}(\mathbf{k}',\omega+\omega'))$$

The formula for the local density approximation of $\Sigma(\mathbf{n}(\mathbf{r}))$:

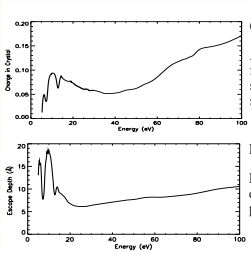
$$\begin{aligned} \mathrm{Im}(\Sigma) &= a/(1.+\exp(-(E-\phi_s-w_p)/E_f))+d \\ \text{with} \\ E_f &= 13.6\frac{3.683}{r_s^2}, \quad \text{Fermi energy} \\ r_s &= [\frac{3}{4\pi n(\mathbf{r})}]^{1/3} \\ w_p &= 13.6\sqrt{12/r_s^3}+E_f, \quad \text{plasma frequency} \\ d &= 0.12E_f \\ a &= \max[(0.3r_s-0.24)E_f-d,0.) \end{aligned}$$

- Stronger damping at high energies than expected
- Escape depth modulated by band structure
- Escaping wave characterized by one dominating wave vector

Escape Depth and Energy



- Below the plasma frequency the escape depth is strongly dependent on the band structure.
- Density dependent Σ creates structures at a Bragg gap



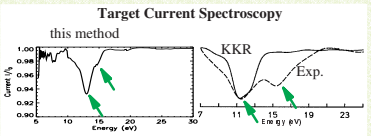
Charge in crystal

Another criterion for surface sensitivity shows similar structure

Escape depth

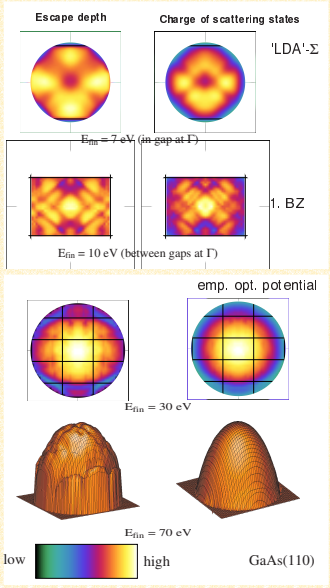
For comparison : empirical optical potential

Target Current Spectroscopy



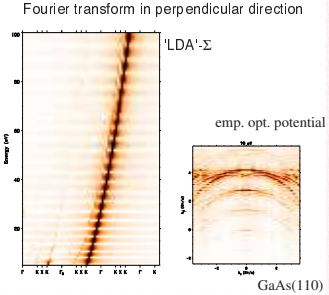
URL: http://www.tp.cau.de/schattke/

Sensitivity in Momentum Space

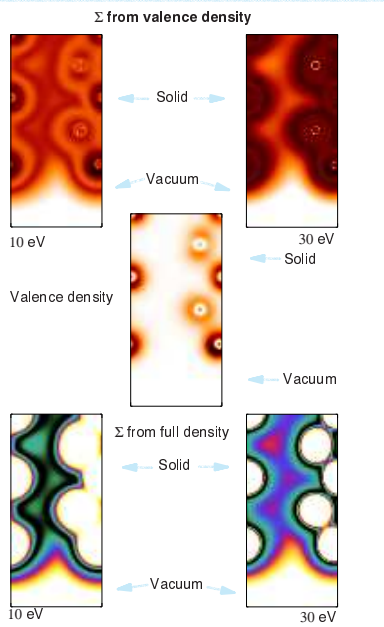


- Band structure effects, especially the gaps, are pronounced
- Escape depth (exponent) in comparison with charge underestimates the surface sensitivity at large angles.

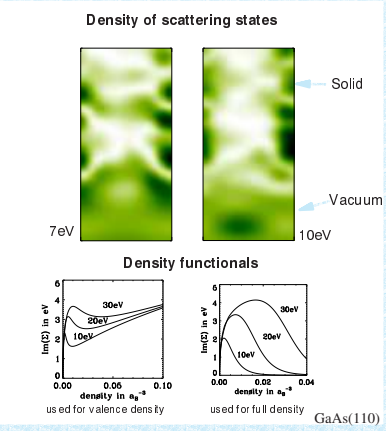
Perpendicular Wave Vector



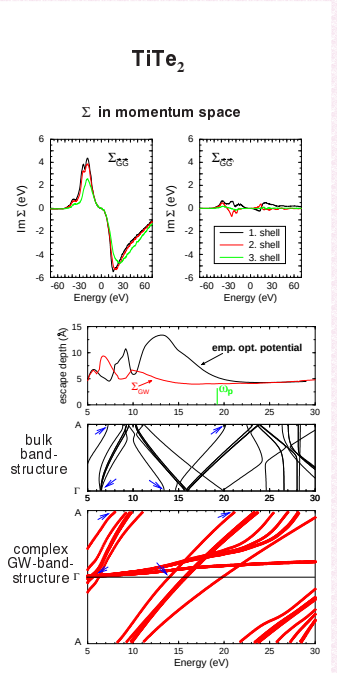
LDA-like Model for Σ



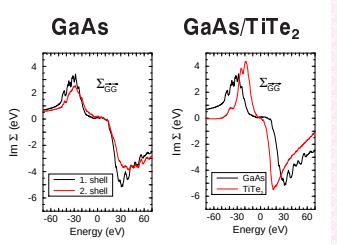
- Im(Σ) is calculated from the valence density (upper) resp. the full ground-state density.
- In the vicinity of atoms the damping is low, because the high density yields a high 'local Fermi energie'



GW-Σ



- GW-Σ is bigger than the heuristic one → escape depth is smaller
- ImΣ shifts the bands as the arrows mark
- ImΣ is almost diagonal → in real space ImΣ depends on r-r'



- GaAs has a richer band structure, so Σ shows more modulations