Revealing surface information with atomic resolution secondary electron imaging

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Introduction

With the development of aberration corrector, nowadays we can observe materials in real space with atomic resolution. TEM with high energy electron is a powerful tool to get atomic resolution, but we usually use angular dark field (ADF) detector to collect electron transmits through the material, surface information is covered. On the other hand, secondary electron (SE) has low energy that below 50 eV, only SE ejected from surface can reach detector, thus is a common way to get surface information. But traditionally, SE image is obtained in SEM, spatial resolution is limited.

Recently, using aberration corrected TEM, Zhu et al was able to demonstrate atomic resolution SE imaging of $YBa_2Cu_3O_{7-x}$ superconducting crystal[1], In 2018 H.G. Brown et al gave a quantum model of secondary electron ionization form factor [2] :

$$F(Q,\kappa) = \frac{4\pi}{\kappa} \sum_{l'=0}^{\infty} \sum_{m_{l'}=-l'}^{l'} (-i)^{l'} e^{-i\delta_{l'}} Y_{l',m_{l'}}(\kappa) \times \sum_{\lambda=0}^{\infty} \sum_{m=-\lambda}^{\lambda} i^{\lambda} Y^{*}_{\lambda,m_{\lambda}}(Q) \int \frac{1}{r^2} u_{\kappa l'}(r) j_{\lambda}(2\pi Q r) \times u_{\nu l}(r) Y^{*}_{l',m_{l'}}(\hat{\mathbf{r}}) Y_{l,m_l}(\hat{\mathbf{r}}) Y_{\lambda,m_{\lambda}}(\hat{\mathbf{r}}) d\mathbf{r}$$

$u_{\nu l}(r)$ and $u_{\kappa l'}(r)$ is SE initial and final state wave function, calculated using a self-consistent Dirac-Fock-Slater iteration. This theoretical model, combining with multi-slice simulation, we can explain more SE image contrasts that reveals physical properties.

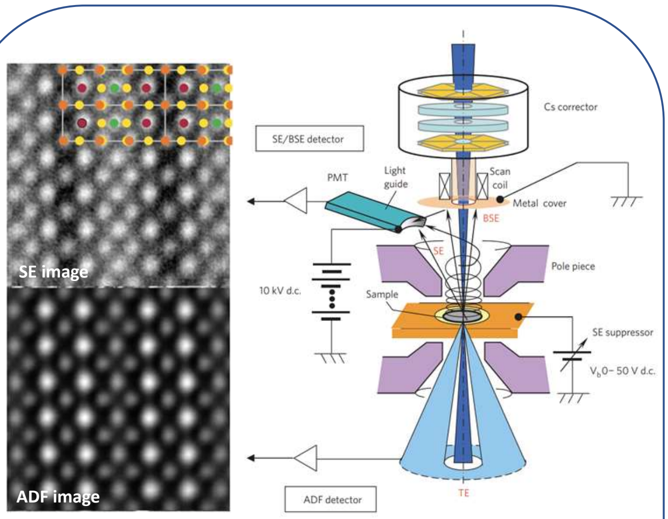


Figure1. Right is experiment setup of STEM with ADF detector and SE detector. Left is ADF image and SE image of $YBa_2Cu_3O_{7-x}$, strips along Yttrium can be see on SE image.

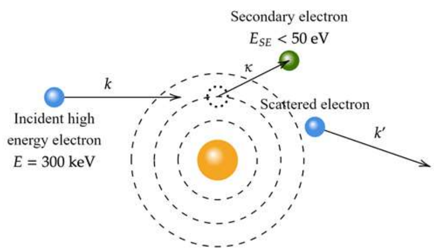


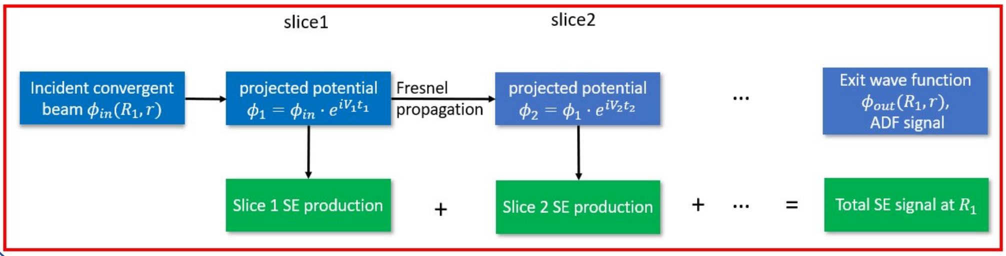
Figure2. Emission of secondary electron

Secondary electron multi-slice simulation

Differential scattering cross section can be calculated from ionization form factor, then SE production is:

$$SE = 2\pi \int \frac{\partial\sigma}{\partial\Omega_\kappa}|_R \, exp\left[-\frac{z}{l(E_\kappa)\cos(\theta_\kappa)}\right] d\Omega_\kappa$$

l is mean free path for SE. For every beam scanning position, repeat the calculating process of the chart below, we can obtain simulated ADF and SE images.



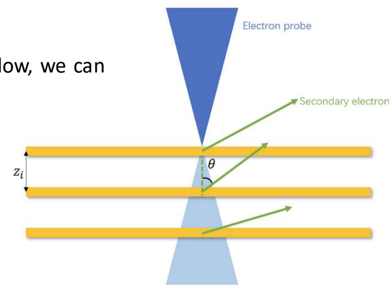


Figure3. Schematic figure of probe dynamic scattering and SE ejected at each slice.

Result

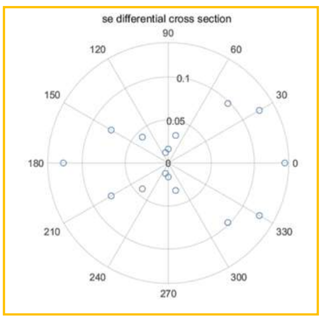


Figure4. Calculated differential cross section, assuming plane wave incident from the left, SE ejected from 1s

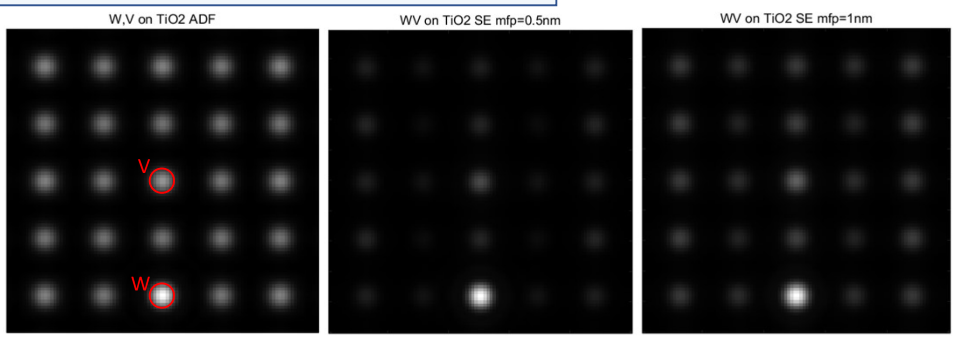


Figure5. Simulation image of single atom catalyst W, V on TiO_2 [001]. W is obvious in both cases because of it's high Z number. Meanwhile, V can hardly be seen in ADF image, but in SE image V has better contrast. Mean free path (mfp) has a great influence on SE contrast.

Reference

[1] Y. Zhu, H. Inada, K. Nakamura, and J. Wall, Nat. Mater. 8, 808 (2009).

[2] H. G. Brown, A. J. D'Alfonso, and L. J. Allen Phys. Rev. B 87, 054102 (2013).