Dynamical Simulations of Transmission Kikuchi Diffraction Patterns

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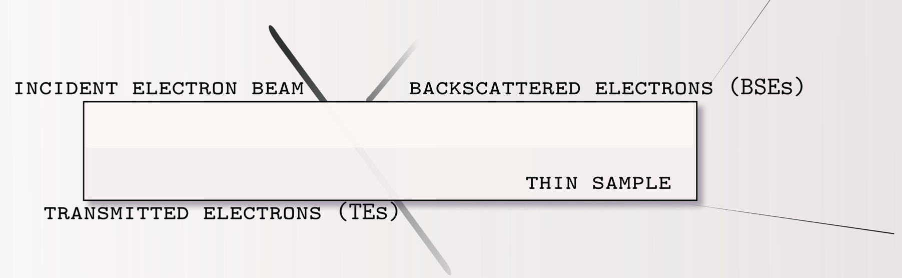
Background

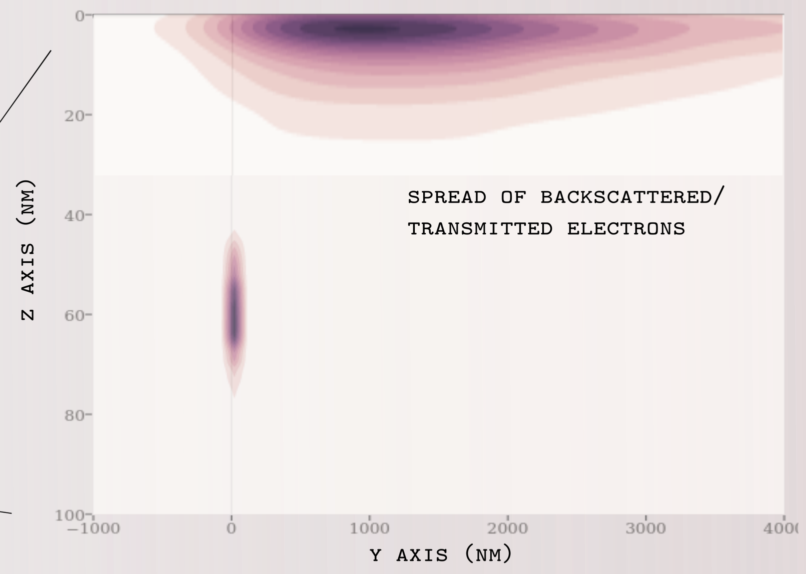
The spatial resolution of EBSD is dictated by the interaction volume of those electrons that carry diffraction information on their way out of sample to produce Kikuchi patterns on the detector. In conventional geometry these are the backscattered electrons which can travel a significant distance before escaping the sample, 'sampling' a rather broad interaction volume.

The idea of questioning instead the electrons transmitted through a thin sample for diffraction information as a method of improving the lateral spatial resolution has attracted considerable attention [1,2]. In this case the detector is placed on the other side of a thin sample and transmission Kikuchi diffraction patterns are collected.

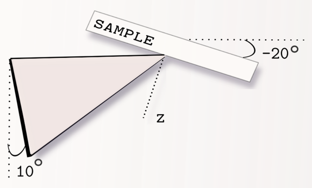
Following previous diffraction patterns simulations for EBSD [3], the prediction of diffraction patterns in general involves a double integral: over the energy range of and over the distance travelled on their way out by the escaping electrons. Monte Carlo simulations of electron scattering processes inside the sample can be used to estimated the energy and depth distributions of the incoherent point sources [4].

Interaction volume of backscattered and transmitted electrons shown here as kernel density estimates plots of the escaping electrons. The position of escaping electrons is assumed to be the last scattering event before exiting the sample. The data was produced from Monte Carlo simulations using Casino [5] software for an incident beam of 30 keV on a 70°/ 20° tilted sample of thin Silicon. Different sample thicknesses are used in order to produce the same total number of backscattered and transmitted electrons.

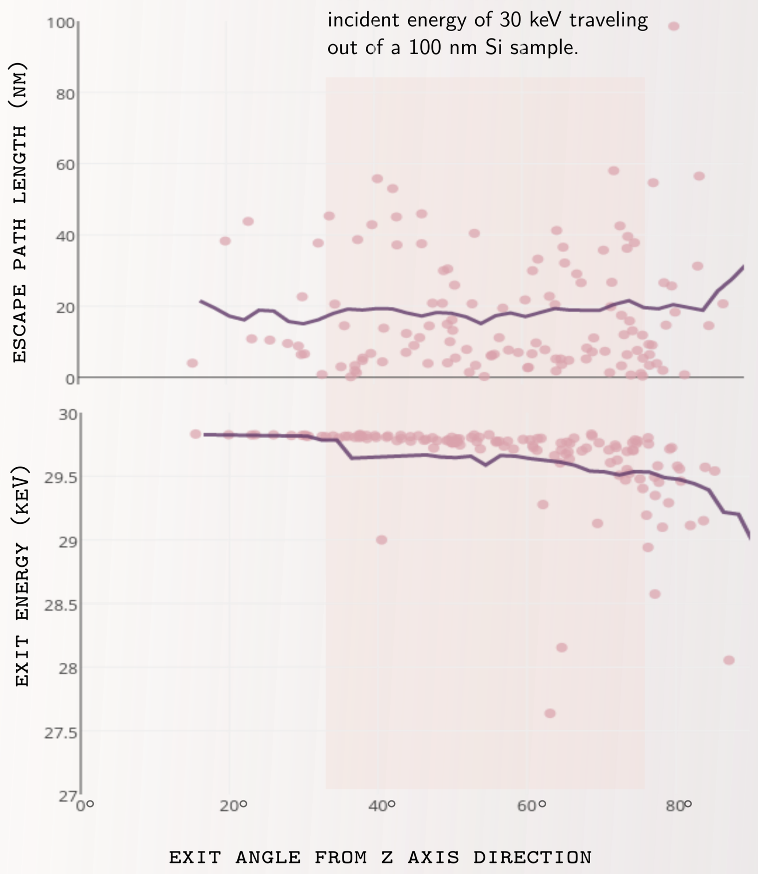




Dynamical electron scattering



In standard TKD geometry the path lengths and energies of electrons that reach the detector does not show strong dependency on the exit angle. Below are MC results for 50k electrons with incident energy of 30 keV traveling out of a 100 nm Si sample.



The probability for an electron to be emerging from the sample in a direction **k** can be written as follows:

$$P(\hat{\mathbf{k}}) = \sum_{n \in \text{A.U.}} P_n(\hat{\mathbf{k}})$$

where the sum goes over all positions in the asymmetric unit (A.U.) and

$$P_n(\hat{\mathbf{k}}) = \sum_{j \in \mathcal{S}_n} \sigma_j \int_{E_{\min}}^{E_{\max}} \mathrm{d}E \int_0^{z_0(E)} \mathrm{d}z\, \bar{\lambda}_{\hat{\mathbf{k}}}(E,z) |\Psi_{\hat{\mathbf{k}}}(\mathbf{r}_j; E, z)|^2. \quad (1)$$

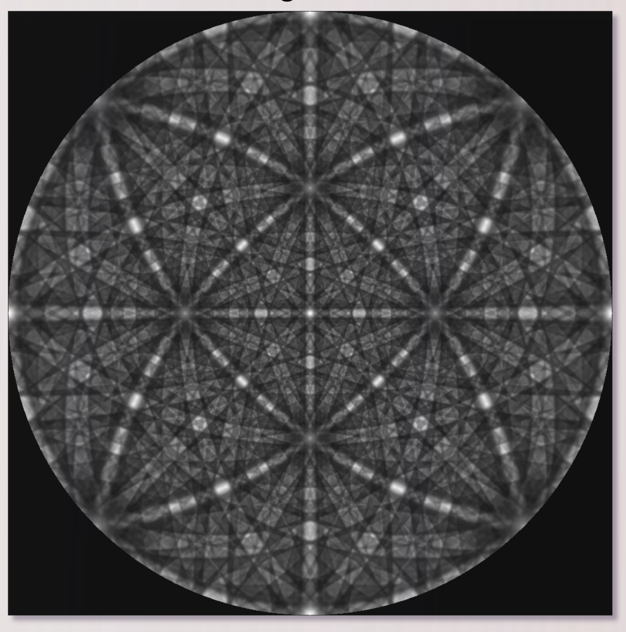
with σ_j the Rutherford scattering cross section for atom *j* in the set of equivalent positions *Sn;*

$\bar{\lambda}_{\hat{\mathbf{k}}}(E,z)$ a weighting function which can be derived from Monte Carlo distribution simulations and for which to a good approximation the direction dependence can be averaged over:

$$\bar{\lambda}_{\hat{\mathbf{k}}}(E,z) \rightarrow \bar{\lambda}(E,z)$$

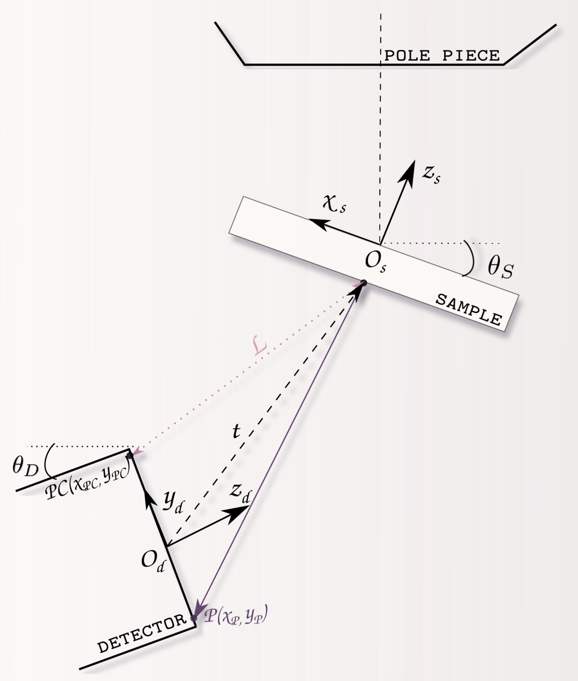
and the wave function $\Psi_{\hat{\mathbf{k}}}$ evaluated for the equivalent atom positions $\mathbf{r}_j$ using the scattering matrix formalism for a scattering direction **k**.

If the probabilities are calculated for all independent scattering directions a 'master TKD pattern' is obtained from which any needed TKD patterns can be extracted via bi-linear interpolation. This method reduces the number of calculations needed for a specific set of patterns as the multibeam dynamic simulations must only be carried once for all beam directions.



Master TKD pattern for all possible independent exit directions in the Northern hemisphere using equal area Lamber projection. The simulation was done for 100 nm thick sample of Ni and a beam energy of 20 keV using the EMsoft v3.1 package [6].

Geometry



TKD Geometry where *PC* is denotes the pattern center and *L* is the distance between the detector and the sample.

Following the EBSD experimental geometry described by Callahan [3] we can derive the TKD sample-detector coordinates transformation.

For a translation vector ***t*** which moves the origin of the detector frame O_d to the origin of the sample frame O_s defined as:

$$t = (x_{PC}, y_{PC}, L)$$

the coordinates of a point P(x_P, y_P) on the detector in the reference frame of the sample can be derived geometrically:

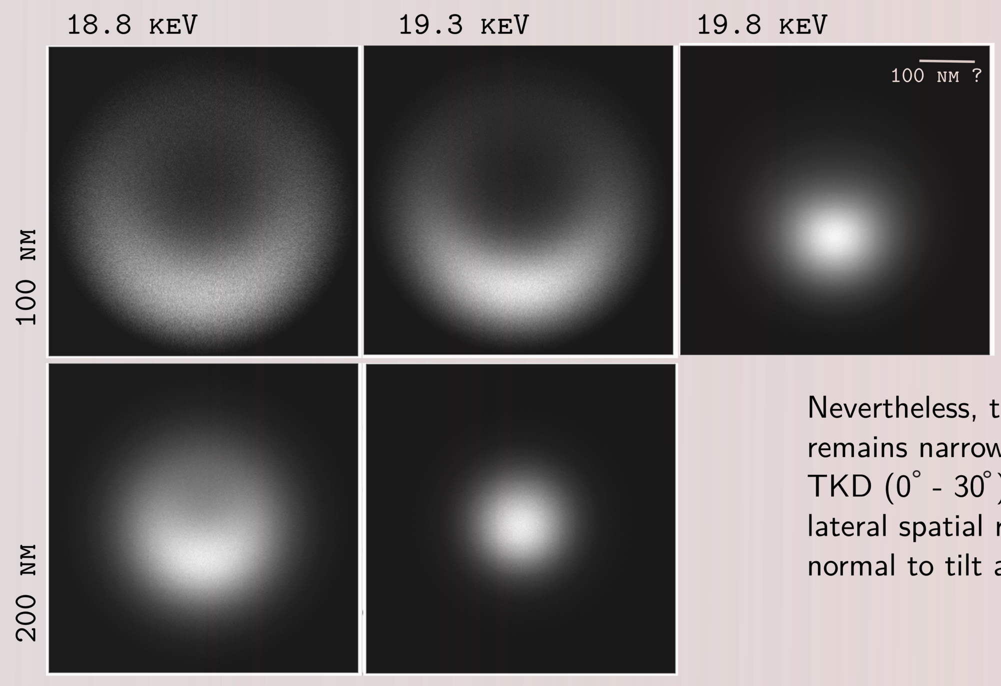
$$\vec{O_s P} = \mathcal{R}^{ds}\left(\vec{O_d P} - \vec{t}\right)$$

where $\mathcal{R}^{ds}$ is the coordinate transformation from the sample frame to the detector frame. Such that finally the direction cosines of a pixel on the screen in the sample frame is:

$$P^s = \begin{bmatrix} -\cos\alpha(y_d - y_{PC}) + L\sin\alpha \\ -(x_{PC} - x_d) \\ \sin\alpha(y_d - y_{PC}) - \cos_\alpha(z_d - L) \end{bmatrix} \quad \text{where} \quad \alpha = \pi/2 + \theta_S + \theta_D$$

For a given crystallographic orientation the direction cosines can be converted to the possible channeling out directions the pixels on a detector will register. This can be done for all grains in a sample and the information can be stored in a look up table.

TEs distributions

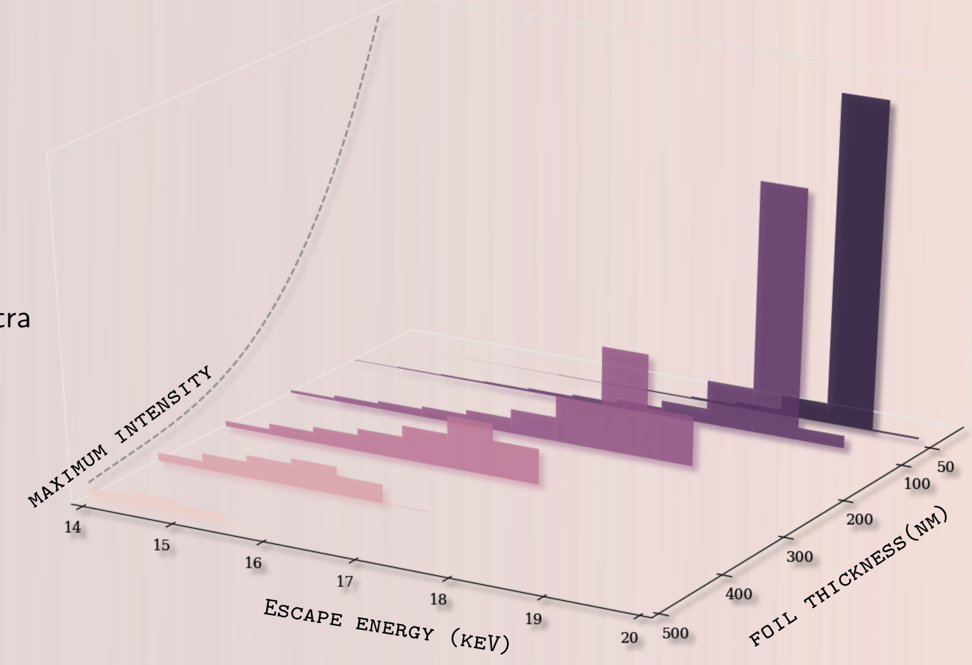


Spatial intensity distributions of escaping electrons at different energies and film thicknesses. The incident beam has 20 keV energy and is incident on a 20° tilted Ni sample. Note the great variation over a narrow range of energies. The inverted intensity distribution for the 100 nm film 18.8 keV bin is due to the fact that the film thickness is comparable to the mean free path.

Similarly to the be intensity distributions in EBSD, the highest energy electrons will follow the incident beam direction and show as an excess of intensity in the lower part of the detector. This effect, however, will be suppressed as the samples thickness is increased.

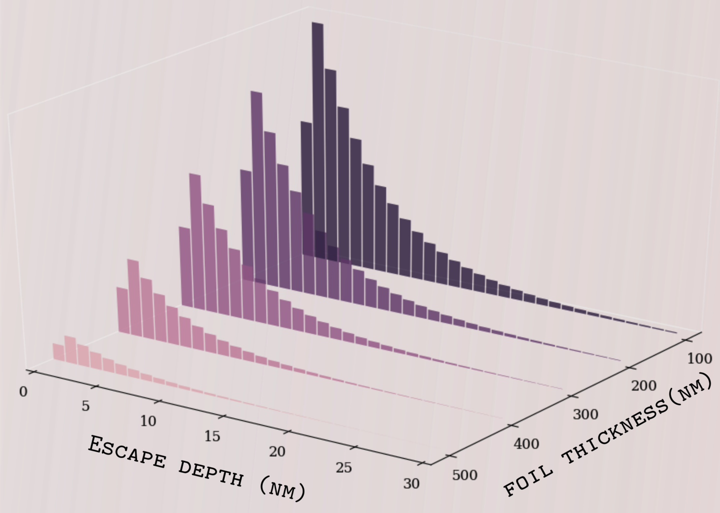
Nevertheless, the spatial distribution of transmitted electrons remains narrow for all energies. Since the conventional sample tilt in TKD (0° - 30°) is so much more shallow than in EBSD (~70°), the lateral spatial resolution is especially improved in the direction normal to tilt axis.

While equation (1) is independent on the diffraction modality (EBSD, ECP, TKD), in the case of TKD an extra weighting parameter must be introduced. The sample thickness affects directly the escaping electrons distributions and their energies.

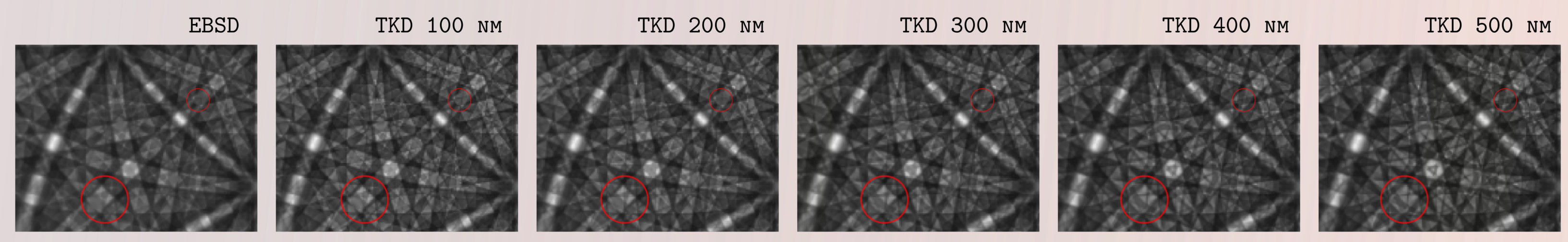


Energy distributions versus sample thickness for electrons exiting a 20° tilted Ni sample. For very thin sample the energy distribution is narrow and we can expect sharp features while for thicker films energy absorption becomes more prominent and distributions will become broader with diffraction lines suffering blurring. The peak of the energy distribution is strongly influenced by sample thickness underlining the requirement for uniform thickness samples in TKD.

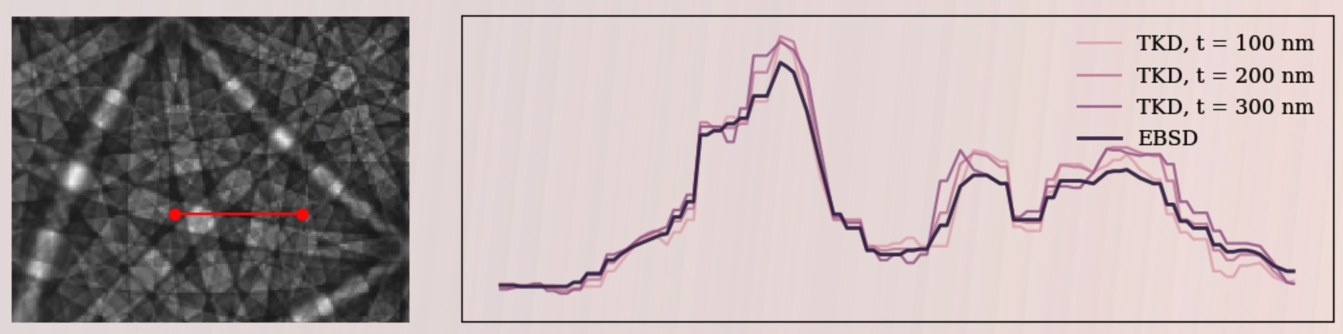
Comparison with EBSD



The narrower energy distributions of the electrons contributing to the TKD pattern shows up as an improvement in the sharpness of Kikuchi lines when compared to the EBSD patterns. This is especially true for the higher order lines which bring a richness of details in the TKD patterns. It is interesting to note that the contrast of these fine features follows more the EBSD pattern values when the sample is thinner. This could be explained by the fact that the escape depth distribution actually becomes broader for thinner samples where not much energy is absorbed from the primary beam and therefore resembling closer the distances travelled by escaping electrons to produce EBSD patterns.



Same area on the Master Pattern comparison between EBSD and TKD for various sample thicknesses. TKD patterns show much finer diffraction details which are very dependent on the sample thickness. The large circle fallows the behaviour of a dark gray feature which vanishes for very thin samples. The smaller circles follow the gain of contrast of a set of higher order Kikuchi lines as the sample thickness is increased.



Intensity line scan (red line on left) comparison between EBSD and TKD patterns simulated for Ni in same sample geometry. The TKD patterns not only show higher contrast features (defined as the difference between maximum and minimum intensity), but also finer details than the EBSD one.

Conclusions and further work

The computational model combining the dynamic scattering theory with Monte Carlo distribution simulations packaged as EMsoft [6] has been expanded to include Transmission Kikuchi Diffraction patterns simulations. This was achieved by implementing a Monte Carlo algorithm in the TKD geometry which tracks electrons exiting from the bottom of the sample. This in turns implies that the probability distributions of diffraction carrying electrons will depend on the sample thickness in addition to the other parameters present for the other diffraction geometries.

The relationship between the probability distributions predicted by Monte Carlo simulations which use empirical parameters usually verified for behaviour outside the sample and the distribution of 'sources' of coherent electrons inside the sample will be reviewed in future work.

References

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EPSRC Engineering and Physical Sciences Research Council
NPL National Physical Laboratory
SUPA