Dynamical Diffraction in High Energy Electrons by Light-Atom Structures : A Multiple Forward Scattering Interpretation

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Abstract

Due to the strong electron-atom interaction, the kinematic theory of diffraction can not be used to describe the scattering of electrons by an assembly of atoms. Dynamical diffraction need to be taken into account by solving Schrödinger's equation. In this paper, the scattering of high energy electrons by a regular array of light atoms is solved exactly using the T-matrix in spherical coordinates. Using the independent atom model, each atom is represented by a sphere with an effective constant potential. The validity of the forward scattering approximation and the phase grating approximation assumed by the popular multislice method are discussed. An interpretation of multiple scattering is proposed and compared with existing interpretations.

Keywords: High Energy Electron Diffraction, T-matrix

1. Introduction

1.1. Motivation

Since the first experimental demonstration of electron diffraction in 1928, theory of dynamical diffraction has been developed [1, 2]. Besides, multiple scattering [3, 4, 5, 6] has also extensively been studied in solid state physics over the 20th century. In fact, even at very high electron energies commonly used in modern transmission electron microscopes, the electron-atom interaction is very strong and the the kinematic theory of diffraction is not theoretically valid for crystals thicker than a few nm[7, 8]. In practice, crystal growth cannot be controlled to such a degree of accuracy and nano-crystals of organic compounds are usually on the order of tens to hundreads of nanometers. This is known as a challenging aspect of high energy electron diffraction (HEED) as it should significantly complicate the structure determination process. However, successfull structure determination based on the standard kinematic theory used in X-ray diffraction have regularly been demonstrated over the past 10 years[9, 10] suggesting that dynamical diffraction may not affect the diffraction intensities as much as the theory suggests. Although, dynamical refinement based structure determination [11] usually leads to better intensity predictions [12], the agreement between theory and experiment is still significantly worse than those obtained for X-rays [13]. It is therefore crucial to develop more accurate models of electron diffraction by crystals.

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1.2. state of the art

The multislice(MS) [14] and Blochwave(BW) [1] approaches are the most popular methods for simulating scattering of high energy electrons in crystals. The MS is particularly well suited for solving large structures as it involves successive convolutions which can be very efficiently computed with the Fast Fourier Transform(FFT) [15]. To avoid aliasing transverse periodic boundary conditions must be met which is only possible for orthorombic structures in zone axis orientations. Although small beam tilt can also be used [16, 17], simluations with arbitrary orientations must be performed by simulating a full crystal with added zero padding. This can quickly become computationnally challenging.

On the other hand, BW method can simulate small structures in any arbitrary orientations. Although some efficient implementation [18] can simulate moderately large structures, BW cannot be applied to large structures due to the unfavorable scaling behaviour of the matrix diagonalization involved. Non periodic structures, defects and solvent scattering cannot be modelled either.

Both approach can handle coherent inelastic scattering through the use of a imaginary part of the potential. This however does not account for the loss of coherency induced by inelastic scattering which may have dramatic impact on the dynamical diffraction [19].

1.3. Contribution and outline

The purpose of this paper is to propose an alternative real space approach to the scattering of fast electrons by light-atom structures based on the T-matrix formalism. The T-matrix has been extensively applied to various areas of physics including electromagnetics [20, 21, 22],

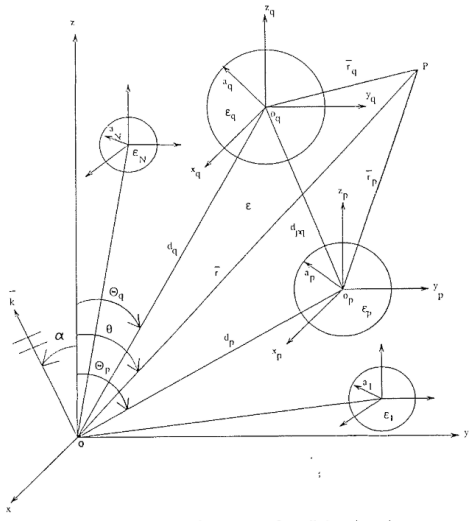


Figure 1: The problem solved by the T-matrix

optics [23] and acoustics [24, 25]. Although not computationnally competitive with multislice for large systems, this approach provides an exact solution to Schr"ødinger's equation for an assemble of spherically symmetric effective atomic potentials in the independent atom model(IAM). An intuitive understanding of multiple scattering in the forward scattering approximation is presented and compared with existing intepretations. The validity of the forward scattering approximation and the phase grating approximation used by multislice are then discussed. Conclusions are drawn and extensions of this approach to account for incoherent inelastic scattering are outlined.

2. Theory

The problem of the scattering of fast electrons by an assembly of atoms is found by solving Schröodinger's equation :

$$\left[-\frac{\hbar^2}{2m_e}\boldsymbol{\nabla}^2_{\mathbf{r}} - eV(\mathbf{r})\right]\Psi = E\Psi \tag{1}$$

where $\hbar$ is plank's constant, m_e the mass of the electron, e the elementary charge, $V(\mathbf{r})$ is the spatially varying electrostatic potential created by the atoms and E the energy of the incident electrons. The wave function is sought as a sum of an incident wave $\Psi^{(i)}$ and a scattered wave $\Psi^{(s)}$.

2.1. T-matrix formulation

In its standard form, the T-matrix solves for the case where the electrostatic potential is uniform constant inside non overlapping spheres and the incident wave is described by a plane wave of wavenumber k_0. The setup shown in figure 1. The formulation is well established and the theory is outlined for the purpose of introducing the forward multiple scattering approximation picture.

in each domain are given by the solutions to the Helmholtz equation in spherical coordinates :

$$\begin{aligned}\boldsymbol{\nabla}^2_{\mathbf{r}_p}\Psi + k_p^2\Psi &= 0\\ k_p &= k_0\sqrt{1+\frac{V_p}{E}}\\ k_0 &= \sqrt{\frac{2m_eE}{\hbar^2}}\end{aligned}$$

where $V_p \geq 0$ is the constant attractive potential inside sphere p of radius a_p centered at $\mathbf{d}_p$. The scattered wave function inside and outside of sphere p can then be expressed as :

$$\begin{aligned}\Psi_p^{(in)}(\mathbf{r}_p) &= \sum_{l=0}^{\infty} j_l(k_p r_p)\sum_{m=-l}^{m=l} a_{p;lm}Y_l^m(\theta_p,\phi_p)\\ \Psi_p^{(out)}(\mathbf{r}_p) &= \sum_{l=0}^{\infty} h_l^{(1)}(k_0 r_p)\sum_{m=-l}^{m=l} b_{p;lm}Y_l^m(\theta_p,\phi_p)\end{aligned}$$

where $p = 1..N$, E, $k_0 = 2\pi/\lambda$ are the energy and wave number of the incident wave, k_p, V_p the wave number and constant potential inside the sphere, j_l and $h_l^{(1)}$ are the spherical Bessel and Hankel functions of the first kind, Y_l^m are the spherical harmonics or order l and azimuthal order m. Note that these equations are expressed in the reference frame of each sphere p hence the use of variable $\mathbf{r}_p$.

The unknown coefficients $a_{p;lm}$, $b_{p;lm}$ are found by imposing the continuity of the wave function and its radial derivative at the surface of each sphere p :

$$\begin{aligned}\Big(\sum_{q=1}^{N}\Psi_q^{(out)} + \Psi^{(i)}\Big)\Big|_{r_p=a_p} &= \Big(\Psi_p^{(in)}\Big)\Big|_{r_p=a_p}\\ \partial_{r_p}\Big(\sum_{q=1}^{N}\Psi_q^{(out)} + \Psi^{(i)}\Big)\Big|_{r_p=a_p} &= \partial_{r_p}\Big(\Psi_p^{(in)}\Big)\Big|_{r_p=a_p}\end{aligned}$$

where $f^{(i)}$ is the incident electron wavefunction and a_p the radius of sphere p.

Using the orthogonality of the spherical harmonics the following linear system yields the unknown coefficients :

$$\begin{aligned}a_{p;lm} &= u_{p;l}c_{lm} + u_{p;l}\sum_{q\neq p}^{N}\\ &\quad\sum_{\nu=0}^{\infty}\sum_{\mu=-\nu}^{\mu=\nu} a^{(out-in)}_{\nu,\mu;l,m}(\mathbf{d}_{pq})b_{q;\nu\mu} \qquad (2)\\ b_{p;lm} &= v_{p;l}c_{lm} + v_{p;l}\sum_{q\neq p}^{N}\\ &\quad\sum_{\nu=0}^{\infty}\sum_{\mu=-\nu}^{\mu=\nu} a^{(out-in)}_{\nu,\mu;l,m}(\mathbf{d}_{pq})b_{q;\nu\mu} \qquad (3)\end{aligned}$$

where the translational addition theorem[26] has been used to express the field scattered by sphere q in the reference frame of sphere p that is $f_q^{(out)}(\mathbf{r}_p)$. This operation involves the coupling coefficients $a_{\nu,\mu;l,m}^{(out-in)}(\mathbf{d}_{pq})$ where $\mathbf{d}_{pq} = \mathbf{d}_q - \mathbf{d}_p$.

The coefficient c_{lm} are related to the incident wave. In the case of a plane wave $e^{j\mathbf{k}_0\cdot\mathbf{r}}$, $j = \sqrt{-1}$, the addition theorem is used to expand the plane wave on the family basis os Spherical Bessel soluions :

$$\begin{aligned} c_{lm} &= 4\pi j^l Y_l^{m*}(\alpha_i, \phi_a)\, e^{jk_0 d_p \zeta_p} \\ \zeta_p &= \sin(\Theta_p)\sin(\Phi_p)\sin(\alpha_i) + \cos(\Theta_p)\cos(\alpha_i) \end{aligned}$$

where d_p, Θ_p, Φ_p being the spherical coordinates of the centre of sphere p in the global coordinate system, $0 \leq \alpha_i \leq \pi$ is the angle of incidence with respect to the $\mathbf{e}_z$ axis, $\phi_i = \pi/2$ since the propagation is in the (y,z) plane and $k_0 d_p \zeta_p$ is the phase factor at sphere p. The different notations as illustrated on figure 1.

The coefficients $u_{p;l}$ and $v_{p;l}$ are expressed as :

$$\begin{aligned} u_{p;l} &= \frac{h_l^{'}(k_0a_p)j_l(k_0a_p) - h_l(k_0a_p)j_l(k_0a_p)^{'}}{j_l(k_pa_p)h_l^{'}(k_0a_p) - n_p j_l^{'}(k_pad_p)h_l(k_0a_p)} \\ v_{p;l} &= \frac{n_p j_l^{'}(k_pa_p)j_l(k_0a_p) - j_l(k_pa_p)j_l^{'}(k_0a_p)}{j_l(k_pa_p)h_l^{'}(k_0a_p) - n_p j_l^{'}(k_pa_p)h_l(k_0a_p)} \end{aligned}$$

where $z_l^{'} = \partial_\rho z_l(\rho)$.

Equations (2,3) can be written in a matrix notation :

$$\big(\mathbf{I} - \mathbf{T}\big)\mathbf{A} = \mathbf{L} \tag{4}$$

where $\mathbf{I}$ is the identity matrix, $\mathbf{A}$ is the unknown vector coefficients, $\mathbf{L}$ the incident wave right hand side and $\mathbf{T}$ is the cross-coupling matrix.

2.2. Far field and scattering cross section

In electron crystallography, the diffraction pattern of particular interest which is recorded in the far field. Using the asymptotic behaviour $h_l^{(1)}(k_0 r_p) \approx (-j)^{l+1}\frac{e^{jk_0 r_p}}{k_0 r_p}$ and since $\theta_p = \theta$,$\phi_p = \phi$ the far field scattering amplitude $f_p(\theta,\phi)$ from sphere p can be written as :

$$f_p(\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}(-j)^{l+1} b_{p;lm} Y_l^m(\theta,\phi) \tag{5}$$

The total scattering amplitude is the sum of the contribution from all individual spheres. Since in the far field, $r_p \approx r - d_p\cos(\theta - \Theta_p)$:

$$f(\theta,\phi) = \sum_{p=1}^{N} f_p(\theta,\phi) e^{-jk_0 d_p\cos(\theta-\Theta_p)} \tag{6}$$

The normalized differential scattering cross section is defined as :

$$\frac{\sigma(\theta,\phi)}{\pi a_p^2} = \frac{4\pi r^2}{\pi a_p^2}\left\|\frac{\Psi^{(s)}(r,\theta,\phi)|}{\Psi^{(i)}(r,\theta,\phi)}\right\|^2 = \frac{4\big|f(\theta,\phi)\big|^2}{(k_0 a_p)^2} \tag{7}$$

where we have used $\Psi^{(s)}(r,\theta,\phi) \underset{r\to\infty}{\approx} \frac{e^{jk_0 r}}{k_0 r} f(\theta,\phi)$.

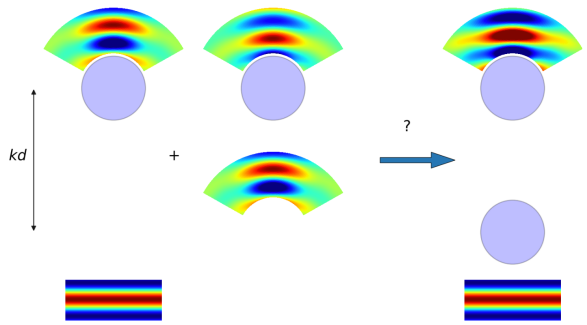


Figure 2: Two-level forward scattering approximation using the T-matrix approach. Neglecting backscattering, scattering from the second scatterer located at distance kd from the first scatterer can be approximated by the sum of 1) the kinematic scattering to the incident beam and 2) the secondary scattering in response to the kinematic scattering from the first scatterer.

3. Forward scattering and multiple scattering approximations

Expression (4) is a convenient way to write the system as it readily identifies $\mathbf{L}$ as the solution to the uncoupled problem. Indeed, $a_{p;lm} = c_{lm}u_{p;l}$, $b_{p;lm} = c_{lm}v_{p;l}$ are them well known analytical solutions of Mie scattering by a soft sphere. Therefore $\mathbf{L}$ represents the kinematic approximation to the solution also known in quantum mechanics scattering theory as the first Born approximation.

The cross-coupling matrix $\mathbf{T}$ accounts for multiple scattering effects. If $\mathbf{A}$ is written $\mathbf{A} = (..a_{p;lm}, b_{p;lm}...)^T$ $\square^T$ denoting transposition, then $\mathbf{T}$ is block diagonal :

$$\mathbf{T} = \begin{bmatrix} \mathbf{0} & .. \mathbf{T}_{1q} .. & .. \mathbf{T}_{1p} .. & \mathbf{T}_{1N} \\ \mathbf{T}_{q1} & .. \mathbf{0} .. & .. \mathbf{T}_{qp} .. & \mathbf{T}_{qN} \\ \mathbf{T}_{p1} & .. \mathbf{T}_{pq} .. & .. \mathbf{0} .. & \mathbf{T}_{pN} \\ \mathbf{T}_{N1} & .. \mathbf{T}_{Nq} .. & .. \mathbf{T}_{Np} .. & \mathbf{0} \end{bmatrix}$$

where $\mathbf{T}_{pq}$ represents the scattering from sphere p due to the scattering from sphere q. If the problem is fully coupled, the scattering from sphere p affects scattering from sphere q and vice versa which therefore requires inversion of the system.

As detailed further down below, backscattering can be neglected for very fast electrons known as forward scattering approximation. This results in $\mathbf{T}$ begin lower triangular if the spheres are sorted in ascending order along $\mathbf{e}_z$. Inversion is therefore no longer necessary and calculations can be performed sequentially.

Since $\mathbf{A}_0 = \mathbf{L}$ represents single scattering, we can establish that $\mathbf{A}_1 = \mathbf{T}\mathbf{A}_0$ accounts for secondary scattering. Similarly, outward scattering ampltiudes rom sphere p can be written :

$$\begin{aligned} b_{p;lm} &= b_{p;lm}^{(0)} + \sum_{q,z_q<z_p} T_{qp} b_{q;lm}^{(0)} \\ &\quad + T_{pq}\sum_{q,z_q<z_p} T_{qr}\sum_{r,z_r<z_q} b_{r;lm}^{(0)} + .. \end{aligned} \tag{8}$$

where the first term accounts for kinematic scattering, the second term for secondary scattering, the third term three time scattering and so on. This is a similar development to the Korringa-Kohn-Rostoker (KKR) theory of multiple scattering [3, 4, 5]. The forward multiple scattering approximation in the case of 2 scatterers is illustrated in figure 2.

3.1. Multiple scattering in multislice

In multislice, the forward scattering approximation is used and the potential discretized in slices which are propagated from one slice to the other using Fresnel propagator. A multiple scattering interpretation by the multislice has been proposed [**?**] which, although analgous to the one presented above, differs in that it is stated in reciprocal space. The expression for the scattering ampltiude $f(h,k)$ of beam h,k is :

$$f(h,k) \propto \sum_{l}\sum_{h_1}\sum_{k_1}\sum_{l_1}..\sum_{h_{N-1}}\sum_{k_{N-1}}\sum_{l_{N-1}} Q_{h_1,k_1,l_1}..Q_{h_{N-1},k_{N-1},l_{N-1}}$$
$$Q\Big(h-\sum_{n}^{N-1}h_n, k-\sum_{n}^{N-1}k_n, l-\sum_{n}^{N-1}l_n\Big)e^{-2\pi j\left(H\zeta-\Delta z\sum_{n=1}^{N-1}\zeta_n\right)}$$

where $h=\sum_{n=1}^{N}h_n$,$k=\sum_{n=1}^{N}k_n$, $H=N\Delta z$ is the total thickness of the sample made of N slices of thickness Δz, $Q_{h,k,l}=-j/\Delta z\delta_{h,k}e^{-2j\pi l_n z_n/c}+\sigma F_{h,k,l}$, $F_{h,k,l}$ is the structure factor, $\sigma=2\pi m_e h/\lambda$ the interaction parameter, ζ the excitation error of beam (h,l) and ζ_n is the excitation error of beam $(\sum_{r=1}^{n}h_r,\sum_{r=1}^{n}l_r)$, and the excitation error is defined as :

$$\zeta=\frac{1}{2K}\Big(\frac{h}{a^2}+\frac{k}{b^2}\Big)-\frac{l}{c}$$

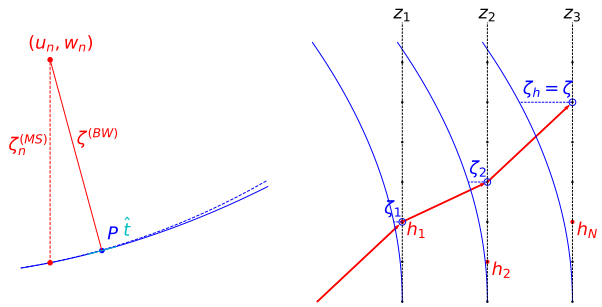
where a, b and c are the lattice constants of the crystal and $K=1/\lambda$ the wave number. This expression is the longitudinal distance of beam (h,k,l) to the Ewald paraboloid which is a very close to the Ewald sphere for large wave vector. This is shown in figure 3a.

The From being scattered n times written only for beams in the zero order Laue zone (ZOLZ) is :

4. Application and Results

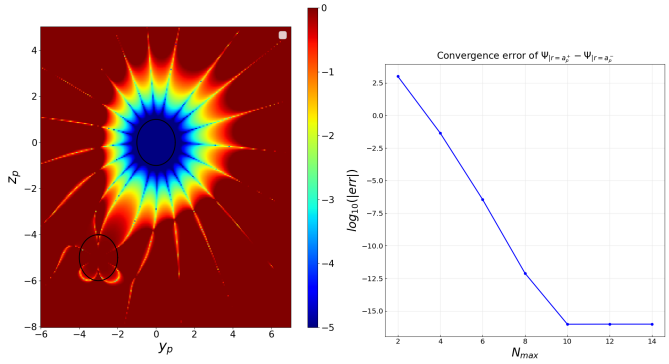
Although very efficient open source implementations are available for electromagnetics [27, 28], an implementation suited for solving Schrödinger's equation has been made available [29].

In practice, the sums over the order l has to be truncated to a integer. A good rule to obtain accurate results is to take l_{max} a few integer above the maximum value of ka. Indeed, the spherical Bessel functions of order l have enough ripples to capture the periodicity of the incident wave in the vicinity of the sphere. Moreover, the translational addition theorem provides an approximation of the spherical Hankel functions with decreasing accuracy from the center at which it is written similarly to a Taylor's expansion. This is illustrated in Figure 4a where the error between $h_l^{(1)}Y_{lm}$ for $l=4$ and $m=2$ computed at the origin and using the translational addition theorem with



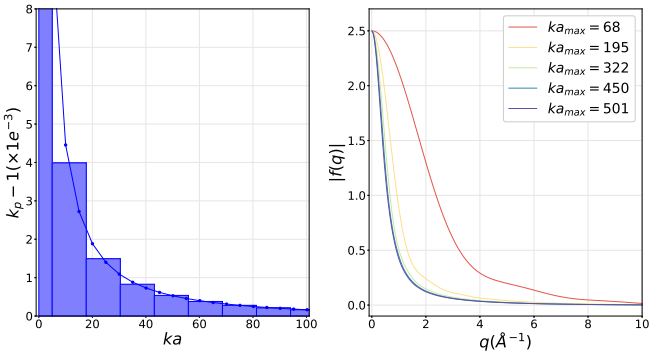
a) b)

Figure 3: Multiple scattering in multislice. a) Distance $\zeta^{(MS)}$ to the Ewald paraboloid(solid curve) as approximated by multislice and distance $\zeta^{(BW)}$ to the Ewald sphere(dashed curve) known as the excitation error in the blochwave theory. Point P is the projection of reciprocal point (u_n,w_n) onto the Ewald paraboloid. b) Multiple scattering in reciprocal space for $N=3$ slices located at z_1,z_2,z_3. The beam is scattered by $h_1,0$, then $h_2,0$ and then $h_N,0$ which results in an overall contribution to reflection h. The open blue circles show the subsequent excitation errors $\zeta^{(i)}$.



a) b)

Figure 4: a) Error between $h_l^{(1)}Y_{lm}$ for $l = 4$ and $m = 2$ computed at the origin and using the translational addition theorem $\mathbf{d}_p = (0, 3, 5)$ with $\nu_{max} = 10$. The circle represent spheres of radius 1. Color axis in logscale. b) Continuity error at the sphere boundaries in the T-matrix with increasing order. For this example $N = 4$ and $ka_{max} = 4$.



a) b)

Figure 5: a) Electrostatic potential created by an atom of carbone. The dashed line shows the Coulomb potential usually used in the IAM using fitted parameteres from [30]. The red solid line shows the best fit using a single screened coulomb potential whereas the blue solid line the best fit using a regular Coulomb potential with offset. The blue patches show a multi-shell approximation model which can be used to represent the potential using a T-matrix approach. b) Scattering amplitude in the Born approximation for the multi-shell model with increasing truncation radius. Although the potential is very small at large radius, a value of $ka_{max} = 325$ is necessary to account properly for the angular spread of the scattering.

$\mathbf{d}_p = (0, 3, 5)$ and $\nu_{max} = 10$ is displayed in logscale. This criteria for selecting l_max is further confirmed by evaluating the continuity of the wave functions at the spheres boundary as shown in figure 4b for $N = 4$ and $ka_{max} = 4$. This can also be used to validate the correctness of the implementation since it can be seen that machine accuracy can be reached with increasing the order.

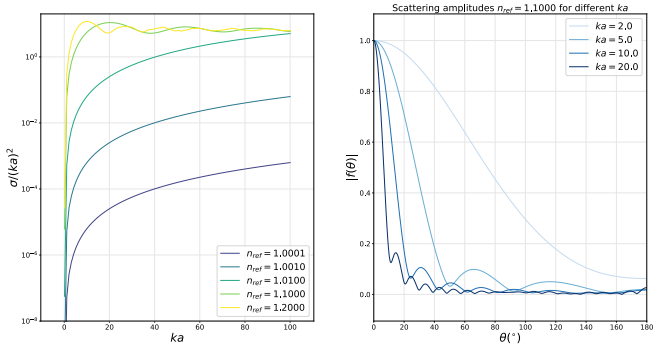
4.1. Validity of forward scattering and phase grating approximation for light atoms

In the case of very fast electrons typically used in transmission electron microscopes $E = 50 - 300keV$. Inclusion of relativistic effects result in $\lambda = 0.025@200keV$ which will be assumed from now on unless stated otherwise. In the IAM, the potential is the sum of the Coulomb potential created by the charge of the nucleus and the electron cloud. It can be approximated with a sum of screened Coulomb potential and Gaussian terms [30]. For typical light atoms such as commonly found in organic compounds, a single screend Coulomb potential term can be a pretty good approximation as shown in figure 5a. The solution to Schrodinger's equation in such a potential can only be solved perturbatively [31] and is beyond the scope of this document. However, orders of magnitude for k_p and ka_p can be estimated by a multi-shell representation as shown in figure 5a. Although the range of the potential is theoretically infinite, it can reliably be truncated to radius ka by using the Born approximation. In figure 5b the multi-shell scattering amplitudes are shown for increasing values of truncation radius. A satisfactory agreement with the electron diffraction scattering factors is obtained for normalized raidus as large as $ka = 350$ to account for the proper low angle representation although the potential is very small at such a radius. As it was seen above, such a large radius would be quite hard to simulate with the T-matrix due to the large orders to be included. However, it can be argued that in the interest of the multiple scattering interpretation presented in this paper, appreciable multiple scattering

4.2. Multiple scattering approximations

It is noted that in the weak scattering regime $kp-1 \ll 1$ and not too large spheres ka, the shape of the diffraction pattern is identical to the Born approximation. Only the amplitude of the scattering cross section increases with radius.

Both the uncoupled and forward scattering approximation work better with increasing distances kd since scattering from the spheres reduces with distance. It is therefore less likely to affect scattering from the other spheres. The



a) b)

Figure 6: a) Normalized scattering cross section in σ in logfor a few values of k_p over a range of normalized radius ka. b) Scattering amplitude for a few normalized radius ka and potential strength k_p.

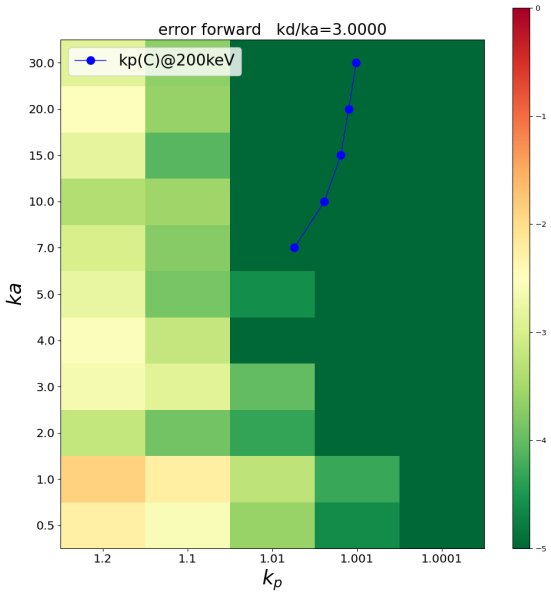


Figure 7: (ka, k_p) map(color axis in logscale) of the error of $b_{p;lm}$ using the forward scattering approximation. The blue dot correspond to the location of the spherical shells of Carbone atom at $E = 200keV$.

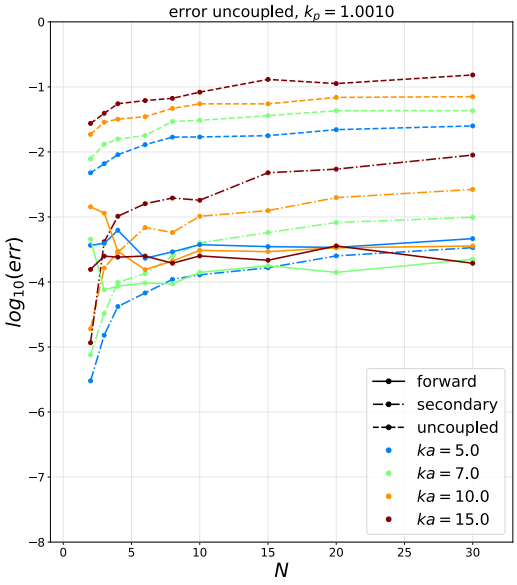


Figure 8: $\log_{10} err(b_{p;lm})$ the scattering amplitudes coefficients with increasing number of spheres for a few normalised radius ka using $k_p = 1.01$.

low values of k_p result in overall good approximation of both the uncoupled and forward scattering approximation. This is an anticipated result since for weak potentials, the kinematic approximation is more valid. The uncoupled approximation improves with small radii since Small ka result in small scattering cross section, On the other hand the forward scattering approximation improves with larger values of ka since backward scattering is less likely for large ka.

5. Conclusion

An alternative approach based on the T-matrix has been applied to the scattering of fast electrons by light-atom structures. The validity of important approximations used in multislice has been discussed and a multiple scattering approximation framework has been proposed and compared to other existing interpretations.

Although the spherically symmetric effective potential does not accurately model the potential used in atoms, it was shown that the multiple scattering interpretation should equally apply to the more accurate case of a screened Coulomb potential. A possible inclusion of such a potential could be performed by using a family of basis functions consistent with the exisiting variational based solutions of the Schrodinger's equation in a Yukawa potential. The main ultimate limitation of both this approach and the traditional multislice lies in the use of the independent atom model which by definition ignores the effect of bonding which may be relevant for structure determination of

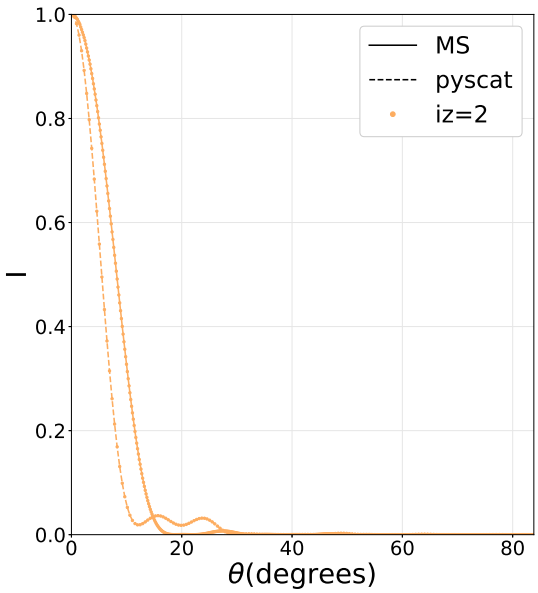


Figure 9: Comparison of multislice and Tmatrix for increasing number of spheres N. $keV = 50$, $ka = 11$, $kd = 3ka$, $k_p = 1.001$.

organic structures. However, it is still an open question whether such bonding play an important role in HEED.

The advantage of a multiple scattering approximation approach is that it offers both the possibility of a massively parallel computation of dynamical diffraction while including incoherent inelastic scattering with a stochastic approach. It is indeed strongly anticipated that inelastic scattering has a dramatic mitigation effect of dynamical diffraction even when energy filters are used.

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