Inverse Elastic Scattering with Adaptive FE Meshes

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Introduction

Here we have addressed the case of elastic scattering as it occurs in Transmission Electronic Microscopy (TEM). Our main goal is to determine the atomic structure of a sample given the electronic wave it diffracts.

In the forward problem, we assume that the potential created by the sample is known at the electronic scale, and the diffracted wave function is calculated at the output of the sample by means of an efficient Finite Elements (FE) computation.

In the inverse problem, the diffracted wave function is measured experimentally, and the unknown potential associated with the sample is sought after using an iterative strategy based on FE mesh adaption.

Theoretical framework of the forward electronic scattering problem

The incident electron is classically considered as a planar wave function $\psi_i(\mathbf{x}) = \tilde{\psi}_i \exp(\mathrm{i}\mathbf{k}_i \cdot \mathbf{x})$ associated with a wave vector $\mathbf{k}_i$. In an infinite, empty domain Ω_e, this wave function should verify the following Schrödinger equation expressed in atomic units (a.u., i.e. distances in Bohr and energies in Hartree)

$$-\frac{1}{2}\Delta\psi_i = E_i\psi_i$$

where $E_i = ||\mathbf{k}_i||^2/2$ is the energy of the incident electron and Δ is the Laplacian operator.

The sample's spatial domain Ω_s is characterized by a potential V, associated with the electrons and nuclei of the sample, which outside decreases rapidly.

By introducing several classical but nonrestrictive assumptions regarding the different energies involved in the problem, the diffracted wave function ψ_d, which is defined as the difference between the whole electronic wave function ψ_e and the incident wave function ψ_i, should verify the following Helmholtz equation:

$$\frac{1}{2}\Delta\psi_d + E_i\psi_d = V\psi_i \qquad (1)$$

If the defects of the microscope's lenses are not taken into account, the square modulus of the whole electronic wave function $||\psi_e||^2 = ||\psi_i + \psi_d||^2$ is directly obtained on a virtual plane Σ_m located at the output of the sample Ω_s, as it is depicted in Figure 1.

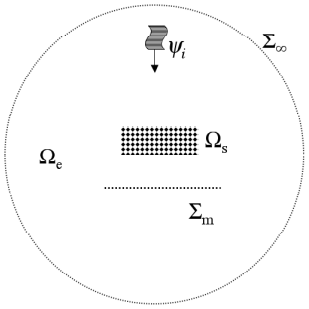

Figure 1. Considered spatial domain.

FE implementation of the forward electronic scattering problem

The use of the FE method should make the resolution of the forward problem for any kind of specimen possible, including specimens with defects or lacunae.

The first difficulty is how to deal with the empty domain, which should be infinite. To circumvent this, we assume that the diffracted wave function is of the evanescent kind far from the specimen. This way we can introduce a boundary Σ_∞ for Ω_e such that, on Σ_∞:

$$\frac{\partial\psi_d}{\partial\mathbf{n}} = \mathrm{i}||\mathbf{k}_i||\psi_d \qquad (2)$$

where $\mathbf{n}$ is the outer unit normal of the boundary Σ_∞ [1].

The second difficulty lies in the high frequency aspect of the problem to solve. Considering estimates of the incident wavelength and of interatomic distances within the specimen, the computation of even one single crystalline cell would require about one billion DOFs to get sufficiently accurate results. So we have introduced a paraxial approximation to drop the computation costs.

Paraxial approximation

The paraxial approximation consists in finding the unknown $\tilde{\psi}_d$ such that:

$$\psi_d(\mathbf{x}) = \tilde{\psi}_d(\mathbf{x}) \exp(\mathrm{i}\mathbf{k}_i \cdot \mathbf{x}) \qquad (3)$$

where $\mathbf{k}_i$ is the incident wave vector, along the microscope's axis in the case of parallel illumination. Important is to stress that this assumption does not necessarily imply that the diffracted wave vectors are close to the $\mathbf{k}_i$-direction, whereas it fits well the experimental TEM.

By using (3) into (1) and (2), we get the following equations to be solved for the forward problem:

$$\frac{1}{2}\Delta\tilde{\psi}_d + \mathrm{i}\mathbf{k}_i \cdot \nabla\tilde{\psi}_d = V\tilde{\psi}_i \text{ in } \Omega_e \tag{4}$$

$$\frac{\partial\tilde{\psi}_d}{\partial\mathbf{n}} = \mathrm{i}(||\mathbf{k}_i|| - \mathbf{k}_i \cdot \mathbf{n})\tilde{\psi}_d \text{ on } \Sigma_\infty \tag{5}$$

Formulation of the inverse problem

The inverse problem consists in determining the potential V spatially-variable in Ω_e such that the intensity $||\tilde{\psi}_i + \tilde{\psi}_d||^2$ of the whole wave function on the virtual plane Σ_m is as close to the measured intensity $||\psi_m||^2$ at the microscope's output as possible. The underlying goal is to be able to locate a defect within the studied sample.

To achieve this, we introduce the following misfit function to be minimized:

$$J(V) = \frac{1}{4}\int_{\Sigma_m}\left(||\tilde{\psi}_i + \tilde{\psi}_d||^2 - ||\psi_m||^2\right)^2 + \frac{\alpha}{2}\int_{\Omega_v}(V - V_0)^2 \tag{6}$$

where α is a regularization parameter to be set, and V_0 a potential chosen *a priori*, such as the potential associated with the perfect crystal in the case of a defect's detection.

This misfit function is minimized by means of an adjoint state method to express the gradient of the misfit function. The adjoint state z verifies:

$$\frac{1}{2}\Delta z + \mathrm{i}\mathbf{k}_i^* \cdot \nabla z = 0 \text{ in } \Omega_e \tag{7}$$

$$\frac{\partial z}{\partial\mathbf{n}} = -\mathrm{i}(||\mathbf{k}_i|| + \mathbf{k}_i^* \cdot \mathbf{n})z \text{ on } \Sigma_\infty \tag{8}$$

$$\frac{1}{2}\left[\left[\frac{\partial z}{\partial\mathbf{n}}\right]\right] = \left(||\tilde{\psi}_i + \tilde{\psi}_d||^2 - ||\psi_m||^2\right)(\tilde{\psi}_i + \tilde{\psi}_d) \text{ on } \Sigma_m \tag{9}$$

where $\cdot^*$ and $[[\cdot]]$ stand for the conjugate and the discontinuity jump respectively.

In this case, the minimization of the misfit function leads to:

$$\mathrm{Re}(\tilde{\psi}_i z^*) = \alpha(V - V_0) \text{ in } \Omega_e \tag{10}$$

The resolution of the inverse problem thus results in solving equations (4) (7) (10) for unknowns $\{\tilde{\psi}_d, z, V\}$ and with boundary conditions (5) (8) (9).

Iterative strategy with adaptive FE meshes

Since the sought potential V is spatially-variable, we choose to apply the strategy described in [2] where the discretization of V is made by means of a FE mesh different from the one used to discretize (4) and (7) . As Bangerth in [3], we stated in [2] that using a coarse mesh to discretize the sought field V and solve (10) behaves as an additional regularization for the inverse problem.

This regularization can be applied in an iterative way, by progressively refining this coarse mesh using classical mesh adaption criteria, thus improving the description of the identified field V.

Example and conclusion

To illustrate this iterative strategy, experimental data are simulated using the equations (4) (5) for a α-iron $2\ \mathrm{nm}$-thick specimen with a single lacuna. This forward problem is solved with 600,000 DOFs in a $200\ \mathrm{keV}$ TEM using a Yukawa's potential [4] for V, depicted as isovalues superposed on the calculated wave intensity on the left of Figure 2.

A first result of identification is presented on the right of Figure 2, depicting the identified discrepancy between the sought potential V and the ideal potential V_0 associated with the crystal with no defect when using the initial coarse mesh for the discretization of V.

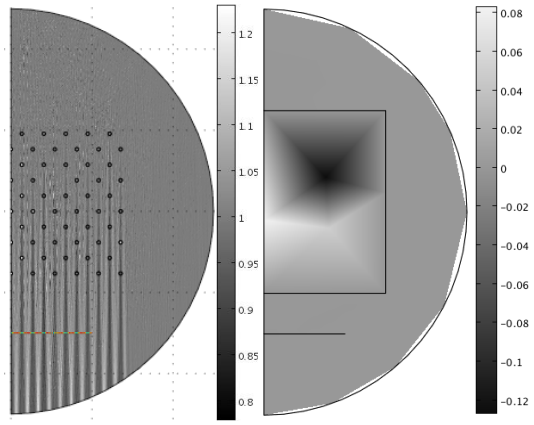

Figure 2. Simulated experimental data (left) and identification of the associated lacuna (right).

Work is on progress about the right choice of the adaption criteria for refining the initial coarse mesh in order to improve the identification of the potential V.

References

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