Software Requirements Specifications (SRS)
STEM Moiré GPA

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1 Revision History

Table 1: **Revision History**

Date	**Version**	**Notes**
xx/xx/xxxx	1.0	First Draft

2 Reference Material

2.1 Table of Units

Throughout this document SI (Système Internationale d'Unités) is employed as the unit system. In addition to the basic units, several derived units are used as described below. For each unit, the symbol is given followed by a description of the unit and the SI name.

Symbol	Base quantity	Name SI
m	length	metre
m^{-1}	reciprocal meter	wave number

2.2 Table of Symbols

The table that follows summarizes the symbols used in this document along with their units if applicable.

Symbol	Unit	Description
$\mathcal{B}_2$		2D orthonormal base in real space
$\mathcal{B}_{2^*}$		2D orthonormal base in reciprocal space
$\mathcal{B}_3$		3D orthonormal base in real space
$\mathcal{B}_{3^*}$		3D orthonormal base in reciprocal space
$\mathcal{B}_C$		3D crystal lattice base
$\mathcal{B}_{C^*}$		3D reciprocal crystal lattice base
$\mathcal{B}_S$		3D orthonormal base in real space defined by the 2D orthonormal sampling scheme
$\mathcal{B}_S^*$		3D orthonormal base in reciprocal space defined by the 2D orthonormal sampling scheme
δ		Dirac delta function
$\mathcal{FT}$		Fourier transform
Γ_{p^X}		Spatial frequency range $[-1/2p, 1/2p]^X$
$\overrightarrow{g_{hkl}}$	nm^{-1}	wave vector associated with (hkl) Miller indices
$\overrightarrow{g_{hkl}}^C$	nm^{-1}	crystalline wave vector with (hkl) Miller indices
$\overrightarrow{g_{hkl}}^M$	nm^{-1}	Moiré wave vector of associated with (hkl) Miller indices
$(G_R^\sigma)_X^C$		List of resolved and allowed crystalline reflections in base X
$(G_R^\sigma)_X^M$		List of resolved and allowed Moiré reflections in base X
i		Imaginary unit
I		Intensity (or number of counts)

Symbol	**Unit**	**Description**
$\mathbb{I}$		Sub-set of $\mathbb{R}$ representing the position of the pixels in an image
$I_{C_{\mathrm{ref}}}$		2D array representing the reference crystal structure
I_{SMH}		2D array representing the experimental SMH
I_{rec}		2D array representing the reconstructed micrograph using the Moiré recovery
M_j		Mask function in Fourier space including the j^{th} wave vector
$\mathbb{N}$		Set of natural numbers
$\vec{\omega}$	nm^{-1}	Vector position in Fourier space
O		Origin of the coordinate system
p	nm	Pixel spacing of the experimental SMH $I_{SMH_{\mathrm{exp}}}$
p_{rec}	nm	Pixel spacing of the reconstructed micrograph I_{rec}
$\overrightarrow{q_{n,m}}$		Sampling vector $\vec{q} \in Q$ of couple $(n, m) \in \mathbb{Z}^2$
Q		Set such that $Q = \{\forall(n, m) \in \mathbb{Z}^2, \vec{q} = n\vec{u_x} + m\vec{u_y}\}$
$Q_{\Gamma_{p^X}}$		Subset of Q including only the sampling vector $\overrightarrow{q_{n,m}}$ shifting the crystalline wave vectors $\overrightarrow{g_{hkl}}^C$ into the Γ_{p^X} spatial frequency range
$\vec{r}$	nm	Vector position
R	nm	Resolution of the STEM probe
$\mathbb{R}$		Set of real numbers
σ		Lattice centering
SMH		2D array representing the experimental STEM Moiré Hologram
$\wedge$		Mathematical symbol for "and"
$\mathbb{Z}$		Set of integer numbers

2.3 Abbreviations and Acronyms

symbol	description
A	Assumption
AU	Arbitrary Unit
DC	Data Constraint
DD	Data Definition
EM	Electron Micrograph
GD	General Definition
GS	Goal Statement
IM	Instance Model
LC	Likely Change
PS	Physical System Description
NR	Non functional Requirement
R	Requirement
SMH	STEM Moiré Hologram
SRS	Software Requirements Specification
STEM	Scanning Transmission Electron Microscopy
T	Theoretical Model

3 Specific System Description

3.1 Problem Description

BLABLA. Terminologies and the physical system are described below.

3.1.1 Terminology and Definitions

- **3D Cartesian coordinate system**: orthonormal coordinate system model by the base $\mathcal{B} = (O, \vec{u_x}, \vec{u_y}, \vec{u_z})$ with O representing the origin and M a point with coordinate the (x, y, z), such that any vector $\vec{r} = \overrightarrow{OM}$ can be expressed as the following :

$$\forall (x, y, z) \in \mathbb{R}^3, \vec{r} = x\vec{u_x} + y\vec{u_y} + z\vec{u_z} \tag{1}$$

- **Pixel**: xxx
- **Electron Micrograph (EM)**: 2D array collected in an electron microscope representing the number of electron crossing the sample (intensity) at each pixel location.
- **Scanning grid**: set representing the succession of the STEM probe positions when collecting the STEM EM. Equivalently the scanning grid represents the relative position of the pixel with respect to the sample when acquiring the EM. A simplified version of the STEM EM formation can be visualized in **??**. The positions of the STEM probe are located at the intersection of the black grid lines.
- **Crystal lattice**: Periodic arrangement of atoms forming matter.
- **STEM Moiré hologram (SMH)**: EM collected in STEM and resulting from the interference between the scanning grid and the crystal lattice.

3.1.2 Physical System Description

The physical system of STEMMoireRec, as shown in **??**, includes the following elements:

- The STEM Moiré hologram as the results of the interaction between the scanning grid and the crystal periodicity of the sample.
- Physical inputs provided by the user to convert a STEM Moiré hologram into strain and rotation maps.

3.1.3 Goal Statements

Given the system description, the goal statement is:

GS 1 Reconstruct an oversampled image from a STEM Moiré hologram

3.2 Solution Characteristics Specification

3.2.1 Assumptions

A 1 The resolution of the microscope cannot resolve any spatial frequency higher than $g_{f_{\text{lim}}}$.

A 2 Only uniform orthogonal and uniform samplers are considered.

A 3 The probe size is smaller than the area covered by one pixel. Therefore, information gathered on one pixel is only provided by the area covered by the pixel (no blurring) and A 1 is the only limiting factor regarding resolution.

A 4 Blabla

3.2.2 Theoretical Models

T 1 2D periodic sampling

- Equation: Equation (3)
- Description: In the 2D Cartesian coordinate system $\mathcal{B}_2$, the scanning grid can be seen as sampler S sampling a continuous function f. In the context of the STEMMoireRec project, the sampler is set to be periodic with the same periodicity p along both $\overrightarrow{u_x}$ and $\overrightarrow{u_y}$ directions (2D Dirac comb). The resulting sampled version f_S of f can be represented as the following with δ representing the Dirac function:

$$\begin{aligned} \forall (x,y) \in \mathbb{R}^2, f_S(x,y) &= S(x,y) \times f(x,y) \\ \forall (x,y) \in \mathbb{R}^2, f_S(x,y) &= \sum_{n=-\infty}^{n=+\infty} \sum_{m=-\infty}^{m=+\infty} \delta(x-np, y-mp) \times f(x,y) \end{aligned} \tag{2}$$

  For shorter notations, it is possible to define a set Q as follows $Q = \{\forall (n,m) \in \mathbb{Z}^2, \vec{q} = n\vec{u_x} + m\vec{u_y}\}$ and thus simplify eq. (2)

$$\forall (x,y) \in \mathbb{R}^2, f_S(\vec{r}) = \sum_{q \in Q} \delta(\vec{r} - p\vec{q}) f(\vec{r}) \tag{3}$$

- Source: [?]
- Ref by: DD 5

T 2 Crystal lattice

- Equation: Equation (4)

- Description: In the 3D crystal lattice coordinate system $\mathcal{B}_C$, the periodic arrangement of a crystalline material in reciprocal space is as follows with $\vec{a}$, $\vec{b}$ and $\vec{c}$ describing the crystal unit cell:

$$\forall(u,v,w) \in \mathbb{Z}^3,\ \overrightarrow{OM}(u,v,w) = \vec{r_C} = u\vec{a} + v\vec{b} + w\vec{c} \tag{4}$$

- Source: xxx
- Ref by: DD 1, DD 3

T 3 Reciprocal crystal lattice

- Equation: Equation (5)
- Description: Reciprocal crystal lattice

$$\begin{cases} \vec{a}^* = \frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})} \\ \vec{b}^* = \frac{\vec{c}\times\vec{a}}{\vec{b}\cdot(\vec{c}\times\vec{a})} \\ \vec{c}^* = \frac{\vec{a}\times\vec{b}}{\vec{c}\cdot(\vec{a}\times\vec{b})} \end{cases} \tag{5}$$

leading the to following reciprocal lattice base $\mathcal{B}_{C^*} = (\vec{a}^*, \vec{b}^*, \vec{c}^*)$ and the expression of the reciprocal lattice $O\vec{M}(h,k,l) = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$

- Source: xxx
- Ref by: DD 2, DD 4

T 4 Reconstruction of a sparse bandwidth-limited periodic function

- Equation: **??**
- Description: Bla
- Source: Our paper
- Ref by: DD 3, IM 3, IM 5

3.2.3 Data Definitions

DD 1 Coordinate of the atoms $\overrightarrow{OM}(x,y,z)$ in the $\mathcal{B}_3$ base,aligning $\vec{u_z}$ to $\vec{c}$ and using $\vec{u_y}$ in the

⋆ Equation: Equation (6)

⋆ Description:

$$\overrightarrow{OM} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \mathcal{M}_{\mathcal{B_C} \to \mathcal{B_\ni}} \begin{bmatrix} u \\ v \\ w \end{bmatrix}$$
$$\text{with } \mathcal{M}_{\mathcal{B_C} \to \mathcal{B_\ni}} = \begin{bmatrix} a \sin\beta \sin\gamma^* & 0 & 0 \\ a \sin\beta \cos\gamma^* & b \sin\beta & 0 \\ a \cos\beta & b \cos\beta & c \end{bmatrix} \text{ and } \begin{cases} \cos\gamma^* = \frac{\cos\alpha\cos\beta - cos\gamma}{\sin\alpha\sin\beta} \\ \sin\gamma^* = 1 - (\cos\gamma^*)^2 \end{cases} \tag{6}$$

⋆ Source: Regarder dans le folder

⋆ Ref by: T 2

DD 2 **Coordinate of the reflection $\overrightarrow{OM}(\lambda, \mu, \nu)$ in the $\mathcal{B}_3$ base,aligning $\vec{u_x}$ to $\vec{a}^*$ and using $\vec{u_y}$ i**

⋆ Equation: Equation (7)

⋆ Description:

$$\overrightarrow{OM} = \begin{bmatrix} \lambda \\ \mu \\ \nu \end{bmatrix} = \mathcal{M}_{\mathcal{B_{C^*}} \to \mathcal{B_\ni}} \begin{bmatrix} h \\ k \\ l \end{bmatrix}$$
$$\text{with } \mathcal{M}_{\mathcal{B_{C^*}} \to \mathcal{B_\ni}} = ({\mathcal{M}_{\mathcal{B_C} \to \mathcal{B_\ni}}}^T)^{-1} \tag{7}$$

,

⋆ Source: Regarder dans le folder

⋆ Ref by:

DD 3 **Type of crystal**

⋆ Equation: Equation (8)

⋆ Description:

$$\begin{cases} (a = b = c) \land (\alpha = \beta = \gamma = 90°) \to \text{cubic} \\ (a = b = c) \land (\alpha = \beta = 90° \ \gamma = 120°) \to \text{hexagonal} \\ (a = b \neq c) \land (\alpha = \beta = \gamma = 90°) \to \text{tetragonal} \\ (a \neq b \neq c) \land (\alpha = \beta = \gamma = 90°) \to \text{orthorombic} \\ (a \neq b \neq c) \land (\alpha = \beta = 90° \ \gamma \neq 90°) \to \text{monoclinic} \\ (a \neq b \neq c) \land (\alpha \neq \beta \neq \gamma) \to \text{triclinic} \end{cases} \tag{8}$$

Permutations of (a, b, c) and (α, β, γ) are also considered

- ⋆ Source: Regarder dans le folder
- ⋆ Ref by: T 2

DD 4 **Simplified reflection (h, k, l) selection rules Ω**

- ⋆ Equation: Equation (9)
- ⋆ Description: Simplified selection rules for existence of the (h, k, l) reflection for some crystal structure S.

$$\begin{cases} \text{Primitive} \rightarrow (h,k,l) \in \mathbb{Z}^3 \\ \text{Body-centered} \rightarrow h+k+l = 2n+1 \text{ with } n \in \mathbb{Z} \\ \text{Face-centered} \rightarrow h,k,l \text{ all odd or all even} \\ \text{Face-centered diamond} \rightarrow h,k,l \text{ all odd or } h,k,l \text{ all even and } h+k+l = 4n \text{ with } n \in \mathbb{Z} \\ \text{Hexagonal closed packed} \rightarrow l \text{ even or } h+2k \neq 3n \text{ with} n \in \mathbb{Z} \end{cases} \tag{9}$$

The only way to be generic is to consider the lattice centering (P, I, A, B, C, F) with the crystal structure to generate the selection rule or look at the group space directly.

- ⋆ Source: Regarder dans le folder
- ⋆ Ref by: T 3

DD 5 **STEM Moiré hologram**

- ⋆ Equation: Equation (12)
- ⋆ Description: The STEM electron micrograph is a 2D array corresponding to the 2D sampling of the crystal lattice I_C with the STEM probe P

$$I_{STEM}(\vec{r}) = \sum_{q \in Q} I_C(\vec{r}) * P(\vec{r}) \times \delta(\vec{r} - p\vec{q}) \tag{10}$$

Using the Fourier series decomposition and assuming that the probe P acts as a simple passband resolving crystalline lattices up to the limit of resolution,

$$\begin{gathered} I_{STEM}(\vec{r}) = \sum_{q \in Q} \sum_{hkl} A_{hkl} e^{2i\pi \overrightarrow{g^C_{hkl}} \cdot \vec{r}} e^{2i\pi \frac{\vec{q}}{p} \cdot \vec{r}} \\ I_{STEM}(\vec{r}) = \sum_{q \in Q} \sum_{hkl} A_{hkl} e^{2i\pi (\overrightarrow{g^C_{hkl}} + \frac{\vec{q}}{p}) \cdot \vec{r}} \end{gathered} \tag{11}$$

If $\vec{q} = \vec{0}$ for all the resolved $\overrightarrow{g_{hkl}}$ then $I_{STEM} = I_C$ and I_{STEM} is the proper discrete representation of I_C. If for at lease one $((h, k, l)$, $\vec{q} \neq \vec{0}$ then $I_{STEM} \neq I_C$ and the

STEM micrograph is an undersampled representation of I_C. In that case, $I_{STEM} = I_{SMH}$ leading to the following expression.

$$I_{SMH}(\vec{r}) = \sum_{q \in Q_{\Gamma_{p^2}}} \sum_{hkl} A_{hkl} e^{2i\pi \overrightarrow{g_{hkl}^{M}} \cdot \vec{r}} \tag{12}$$

- ⋆ Source: Regarder dans le folder
- ⋆ Ref by: T 1

3.2.4 Instance Models

IM 1 List the allowed crystal reflections resolved by the STEM probe

- **Input**: $a, b, c, \alpha, \beta, \gamma, S, R$
- **Output**:$(G_R^\sigma)_{\mathcal{B}_3^*}^C$
- **Description** : For all the resolved reflection ($\|\overrightarrow{g_{hkl}}^C\|_{\mathcal{B}_3^*} < R$), regroup all the allowed reflections ($S \in \Omega$) in G_R^σ expressed in the base $\mathcal{B}_3^*$.
- **Source**: xxx
- **Ref by**: T 2, T 3, DD 3, DD 4

IM 2 Project the crystal reflections in the 3D sampling base $\mathcal{B}_{S^*}$ and keep the reflection in

- **Input**: $(G_R^\sigma)_{\mathcal{B}_3^*}^C$, $\mathcal{B}_S = (\vec{s_x}, \vec{s_y}, \vec{s_z})$ with $\mathcal{B}_\Gamma = (\vec{s_x}, \vec{s_y})$
- **Output**:$(G_R^\sigma)_{\mathcal{B}_\Gamma^*}^C$
- **Description** : For all the reflections in $(G_R^\sigma)_{\mathcal{B}_3^*}^C$, apply the base transformation from $\mathcal{B}_{3^*}$ to $\mathcal{B}_{S^*}$ using the transformation matrix $\mathcal{M}_{\mathcal{B}_{3^*} \to \mathcal{B}_{S^*}}$.

$$(g_{hkl}^C)_{\mathcal{B}_S^*} = \begin{bmatrix} \lambda_s \\ \mu_s \\ \nu_s \end{bmatrix} = \mathcal{M}_{\mathcal{B}_{3^*} \to \mathcal{B}_{S^*}} (g_{hkl}^C)_{\mathcal{B}_S^*} = \mathcal{M}_{\mathcal{B}_{3^*} \to \mathcal{B}_{S^*}} \begin{bmatrix} \lambda \\ \mu \\ \nu \end{bmatrix} \tag{13}$$

All the reflections $(g_{hkl}^C)_{\mathcal{B}_S^*}$ with $\nu_s = 0$ are stored in $(G_R^\sigma)_{\mathcal{B}_\Gamma^*}^C$

- **Source**: xxx
- **Ref by**:T 1, T 3, DD 1, DD 2

IM 3 Spatial frequency shift from Moiré sampling

– **Input**:$(G^\sigma_R)^C_{\mathcal{B}^*_\Gamma}$, p

– **Output**:$(G^\sigma_R)^M_{\mathcal{B}^*_\Gamma}$, $(Q^\sigma_R)^M_{\mathcal{B}^*_\Gamma}$

– **Description** : For all reflection in $(G^\sigma_R)^C_{\mathcal{B}^*_\Gamma}$, the Moiré shift is described using the following equation

$$(g^M_{hkl})_{\mathcal{B}^*_\Gamma} = \begin{bmatrix} \lambda^M_s \\ \mu^M_s \end{bmatrix} = (g^C_{hkl})_{\mathcal{B}^*_\Gamma} + \frac{1}{p}\overrightarrow{q_{n_{hkl},m_{hkl}}}$$
$$\text{with } \begin{cases} n_{hkl} = \lfloor (p\lambda_s - \frac{1}{2}) \rfloor \\ m_{hkl} = \lfloor (p\mu_s - \frac{1}{2}) \rfloor \end{cases}$$

– **Source**: xxx

– **Ref by**:T 4, DD 5

IM 4 Mask all the resolved Moiré reflections from the SMH individually

– **Input**: I_{SMH}, $(G^\sigma_R)^M_{\mathcal{B}^*_\Gamma}$, β

– **Output**:Ψ_{SMH}

– **Description**: For all reflection in $(G^\sigma_R)^M_{\mathcal{B}^*_\Gamma}$, define a mask around the reflection in Fourier space to isolate it from each other

$$\begin{cases} \forall \vec{\omega} = (\lambda, \mu) \in [\lambda^M_s - \beta, \lambda^M_s + \beta] \times [\mu^M_s - \beta, \mu^M_s + \beta], \Upsilon_{hkl}(\vec{\omega}) = 1 \\ \text{else } \Upsilon_{hkl}(\vec{\omega}) = 0 \end{cases} \tag{14}$$

The mask is then applied on the Fourier transform of the STEM Moiré hologram

$$\begin{aligned} I_{SMH}(\vec{r}) &= \sum_{hkl} A_{hkl} e^{2i\pi(\overrightarrow{g^M_{hkl}}\cdot\vec{r})} \\ \tilde{I}_{SMH}(\vec{\omega}) = \mathcal{FT}[I_{SMG}(\vec{r})](\vec{\omega}) &= \sum_{hkl} A_{hkl}\delta(\overrightarrow{g^M_{hkl}} - \vec{\omega}) \\ \tilde{I}_{\Upsilon_{hkl}}(\vec{\omega}) = \Upsilon_{hkl}(\vec{\omega}) \times \tilde{I}_{SMH}(\vec{\omega}) &= A_{hkl}\delta(\overrightarrow{g^M_{hkl}} - \vec{\omega}) \end{aligned} \tag{15}$$

$\tilde{I}_{\Upsilon_{hkl}}(\vec{\omega})$ is regrouped for all reflections in Ψ.

– **Source**: xxx

– **Ref by**: T 4

IM 5 Apply the Moiré correction on each individual reflection and reconstruct the oversam

– **Input**: $(Q^\sigma_R)^M_{\mathcal{B}^*_\Gamma}$, Ψ_{SMH}, p_{rec}

- **Output**:I_{rec}
- **Description**: For each 2D array from Ψ_{SMH}, the opposite of the Moiré shift is applied using the following operation

$$\begin{aligned}\tilde{I}_{\text{rec}_{hkl}}(\vec{\omega}) &= \tilde{I}_{\Upsilon_{hkl}}(\vec{\omega}) * \delta(\overrightarrow{\omega} - \frac{1}{p} \times \overrightarrow{q_{n_{hkl},m_{hkl}}}) \\ \tilde{I}_{\text{rec}_{hkl}}(\vec{\omega}) &= A_{hkl}\delta(\overrightarrow{g^M_{hkl}} - \frac{1}{p} \times \overrightarrow{q_{n_{hkl},m_{hkl}}} - \overrightarrow{\omega})\end{aligned} \tag{16}$$

The reconstruction of the image is performed by summing all the individual Moiré shifted 2D arrays and taking the inverse Fourier transform on the $\Gamma_{p^2_{\text{rec}}} = [-\frac{1}{2p_{\text{rec}}}, \frac{1}{2p_{\text{ref}}}]^2$ spatial bandwidth.

$$I_{\text{rec}}(\vec{r}) = \mathcal{FT}^{-1}[\sum_{hkl} \tilde{I}^{\text{rec}}_{hkl}(\vec{\omega})] \tag{17}$$

- **Source**: xxx
- **Ref by**: T 4

4 Requirements

This section provides the functional requirements, the tasks that the software is expected to complete, and the nonfunctional requirements, the qualities that the software is expected to exhibit.

4.1 Functional Requirements

R 1 Provide an environment for the user to input $a, b, c, \alpha, \beta, \gamma, R$, I_{SMH}, p, $\mathcal{B}_S$ and β.

R 2 Verify $(a, b, c) \in (\mathbb{R}^{+*})^3$, verify $\alpha, \beta, \gamma \in [0, 360[^3$ and verify that S exists.

R 3 Verify I_{SMH} is a 2D array composed of real numbers and check $p \in \mathbb{R}^{+*}$.

R 4 Verify $R \in \mathbb{R}^{+*}$ and assure $(G^{\sigma}_{R})^{C}_{\mathcal{B}^*_3}$ is not empty

R 5 $\mathcal{B}_S$ must be a direct orthonormal base.

R 6 Output all the resolved allowed projected Moiré reflections :$(G^{\sigma}_{R})^{M}_{\mathcal{B}^*_{\Gamma}}$ and let the user asses the match with the experimental data $\tilde{I}_{SMH}$.

R 7 Verify $\beta \in \mathbb{R}^{+*}$ and $\beta < \frac{1}{2p}$

R 8 The Υ_{hkl} must not overlap with each other (only one Moiré reflection $\overrightarrow{g_{hkl}}^M$ per Υ_{hkl} mask)

R 9 Verify $p_{\text{rec}} \in \mathbb{R}^{+*}$, $p_{\text{rec}} > p$ and $\frac{1}{p_{\text{rec}}} > \max_{hkl} \|\overrightarrow{g^M_{hkl}} - \frac{1}{p} \times \overrightarrow{q_{n_{hkl},m_{hkl}}}\|_{\mathcal{B}^*_3}$

R 10 Output I^{rec} to the user

4.2 Non Functional Requirements

NR 1 For the Moiré reconstruction to occur (not be a simple Fourier filtering) at least one crystal reflection $\overrightarrow{g_{hkl}}^C$ must be different from its Moire counter part $\overrightarrow{g_{hkl}}^M$ (at least one sampling vector is non zero $\overrightarrow{q_{n_{hkl},m_{hkl}}} \neq \overrightarrow{0}$).

NR 2 *blbalba*