Software Requirements Specifications (SRS)
STEM Moiré GPA

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Contents

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^S		List of resolved and allowed reflections
i		Imaginary unit
I		Intensity (or number of counts)
$\mathbb{I}$		Sub-set of $\mathbb{R}$ representing the position of the pixels in an image

Symbol	Unit	Description
$I_{C_{\text{ref}}}$		2D array representing the reference crystal structure
$I_{SMH_{\text{exp}}}$		2D array representing the experimental SMH
$I_{SMH_{\text{sim}}}$		2D array representing the simulated SMH
M_j		Mask function in Fourier space including the j^{th} wave vector
$\mathbb{N}$		Set of natural numbers
$\vec{\nu}$	nm^{-1}	Vector position in Fourier space
O		Origin of the coordinate system
p	nm	Pixel size of the experimental SMH $I_{SMH_{\text{exp}}}$
$\overrightarrow{q_{n_j,m_j}}$		Sampling vector $\vec{q} \in Q$ of couple (n_j, m_j)
Q		Set such that $Q = \{\forall (n,m) \in \mathbb{Z}^2, \vec{q} = n\vec{u_x} + m\vec{u_y}\}$
$\vec{r}$	nm	Vector position
R	nm	Resolution of the STEM probe
$\mathbb{R}$		Set of real numbers
σ		Lattice centering
SMH_{exp}		2D array representing the experimental STEM Moiré Hologram
SMH_{sim}		2D array representing the simulated 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 $g_{j_{\text{lim}}}$.

A 2 Uniform orthogonal and uniform samplers are considered.

A 3 Blabla

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 (called pixel size) in both x and 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:

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

  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 2, IM 1, IM 4

T 2 **Crystal lattice**

- Equation: **??**
- 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 3, IM 3, IM 5

T 3 Reciprocal crystal lattice

- Equation: **??**
- 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 $\vec{OM}(h,k,l) = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$

- Source: xxx
- Ref by: DD 3, IM 3, IM 5

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: $\overrightarrow{OM} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \mathcal{M}_{\mathcal{B}_\mathcal{C}\to\mathcal{B}_\ni} \begin{bmatrix} u \\ v \\ w \end{bmatrix}$

with $\mathcal{M}_{\mathcal{B}_\mathcal{C}\to\mathcal{B}_\ni} = \begin{bmatrix} a\sin\beta\sin\gamma^* & 0 & 0 \\ a\sin\beta\cos\gamma^* & b\sin\beta & 0 \\ a\cos\beta & b\cos\beta & c \end{bmatrix}$ and $\begin{cases} \cos\gamma^* = \frac{\cos\alpha\cos\beta - cos\gamma}{\sin\alpha\sin\beta} \\ \sin\gamma^* = 1 - (\cos\gamma^*)^2 \end{cases}$

⋆ Description:

⋆ Source: Regarder dans le folder

⋆ Ref by:

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

⋆ Description:

⋆ Source: Regarder dans le folder

⋆ Ref by:

DD 3 **Type of crystal**

⋆ Equation: $\begin{cases} (a = b = c) \wedge (\alpha = \beta = \gamma = 90°) \to \text{cubic} \\ (a = b = c) \wedge (\alpha = \beta = 90° \ \gamma = 120°) \to \text{hexagonal} \\ (a = b \neq c) \wedge (\alpha = \beta = \gamma = 90°) \to \text{tetragonal} \\ (a \neq b \neq c) \wedge (\alpha = \beta = \gamma = 90°) \to \text{orthorombic} \\ (a \neq b \neq c) \wedge (\alpha = \beta = 90° \ \gamma \neq 90°) \to \text{monoclinic} \\ (a \neq b \neq c) \wedge (\alpha \neq \beta \neq \gamma) \to \text{triclinic} \end{cases}$
Permutations of (a, b, c) and (α, β, γ) are also considered

⋆ Description:

⋆ Source: Regarder dans le folder

⋆ Ref by:

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

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

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

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^σ
- **Description** : For all the resolved reflection ($\|\overrightarrow{g_{hkl}}\|_{\mathcal{B}_3^*} < R$), regroup all the allowed reflections ($S \in \Omega$) in G_R^σ expressed in the base $\mathcal{B}_3^*$.
- **Source**: xxx
- **Ref by**: xxxx

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

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

$$g_{hkl} = \begin{bmatrix} \lambda_s \\ \mu_s \\ \nu_s \end{bmatrix} = \mathcal{M}_{\mathcal{B}_{3^*} \to \mathcal{B}_{S^*}} \begin{bmatrix} \lambda \\ \mu \\ \nu \end{bmatrix} \tag{6}$$

  blbalba
- **Source**: xxx
- **Ref by**: xxxx

IM 3 **Simulate the STEM Moiré hologram imaging formation**

- **Input**: xxxxx
- **Output**:xxxx

- **Source**: xxx
- **Ref by**: xxxx

IM 4 **Mask and transform the Moire reflection into the crystalline one**

- **Input**: xxxxx
- **Output**:xxxx
- **Source**: xxx
- **Ref by**: xxxx

IM 5 **Reconstruct the oversample electron micrograph**

- **Input**: xxxxx
- **Output**:xxxx
- **Source**: xxx
- **Ref by**: xxxx