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
$\mathcal{B}_3$		3D orthonormal base
$\mathcal{C}$		Ceiling function
δ		Dirac delta function
$\Delta\overrightarrow{g_j}^{M_{\text{exp}}}$	nm^{-1}	Variation of the j^{th} Moiré wave vector of SMH_{exp}
$\Delta\overrightarrow{g_j}^{C_{\text{exp}}}$	nm^{-1}	Variation of the j^{th} crystalline wave vector of SMH_{exp}
$\mathcal{FT}$		Fourier transform
Γ		Spatial frequency range
$\overrightarrow{g_j}$	nm^{-1}	j^{th} wave vector
g_{j_x}	nm^{-1}	Component of the j^{th} wave vector along $\vec{u_x}$
g_{j_y}	nm^{-1}	Component of the j^{th} wave vector along $\vec{u_y}$
$\overrightarrow{g_j}^{C}$	nm^{-1}	j^{th} crystalline wave vector
$\overrightarrow{g_j}^{C_{\text{ref}}}$	nm^{-1}	j^{th} crystalline wave vector of $I_{C_{\text{ref}}}$
$\overrightarrow{g_j}^{C_{\text{exp}}}$	nm^{-1}	j^{th} crystalline wave vector of SMH_{exp}
$\overrightarrow{g_j}^{C_{\text{exp}}}_{\text{uns}}$	nm^{-1}	j^{th} crystalline wave vector of SMH_{exp} at its unstrained state
$\overrightarrow{g_j}^{M_{\text{exp}}}$	nm^{-1}	j^{th} Moiré wave vector of SMH_{exp}
$\overrightarrow{g_j}^{M_{\text{exp}}}_{\text{uns}}$	nm^{-1}	j^{th} Moiré wave vector of SMH_{exp} at its unstrained state
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
$I_{C_{\text{ref}}}$		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
∇		Gradient operator
∇u		Displacement gradient tensor
$\vec{\nu}$	nm^{-1}	Vector position in Fourier space
O		Origin of the coordinate system
p	nm	Pixel size of the experimental SMH $I_{SMH_{\text{exp}}}$
p_{ref}	nm	Pixel size of the reference image $I_{C_{\text{ref}}}$
$P_{\overrightarrow{X}}$	rad	2D array representing $2\pi\overrightarrow{X}\cdot\vec{r}$
$\overrightarrow{q_{n_j,m_j}}$		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
$\mathbb{R}$		Set of real numbers
SMH_{exp}		2D array representing the experimental STEM Moiré Hologram
SMH_{sim}		2D array representing the simulated STEM Moiré Hologram
$\vec{u_x}$		Unitary vector from base $\mathcal{B}$
$\vec{u_y}$		Unitary vector from base $\mathcal{B}$
$\wedge$		Mathematical symbol for "and"
$\bigwedge$		Cross product operator
$\mathbb{Z}$		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: ??, IM 1, IM 4

T 2 **Crystal lattice**

- Equation: ??
- Description: In the 3D Cartesian coordinate system $\mathcal{B}_3$, 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: **??**, IM 3, IM 5

T 3 Reciprocal crystal lattice

- Equation: **??**
- Description: Reciprocal crystal lattice

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

- Source: xxx
- Ref by: **??**, IM 3, IM 5

T 4 Reconstruction of a sparse bandwidth-limited periodic function

- Equation: **??**
- Description: Bla
- Source: [**?**, **?**]
- Ref by: **??**, IM 3, IM 5

3.2.3 Data Definitions

DD 1 Variation of the crystalline wave vector $\Delta\overrightarrow{g_j}$ (strain in crystal lattice)

⋆ Equation: Equation (8)

⋆ Description: For the purpose of the STEM Moiré GPA, only mono-crystalline samples are analysed (**??**). In the case of a perfect periodic atomic arrangement, the crystalline lattice I_c can be described in Fourier series with C_j the complex Fourier coefficient related to the crystalline wave vector $\vec{g_j}$ in the 2D Cartesian system $\mathcal{B}$.

$$\forall(x,y) \in \mathbb{R}^2, I_C(\vec{r}) = \sum_{j=-\infty}^{j=+\infty} C_j e^{i(\vec{g_j}\cdot\vec{r})} \tag{6}$$

If the crystal is deformed, the relative position of the atoms will be slightly modified from their original unstrained configuration. The local deformation is breaking locally the perfect periodicity of the crystalline lattice. In the case of small deformation (**??**),

C_j can be allowed to vary in space in eq. (6). Representing C_j with a phase A_j and an amplitude P_j, a pure displacement is only contributing in the phase component. The strain information is therefore embedded in $P_{g_j}(\vec{r})$ such that $P_{g_j}(\vec{r}) = 2\pi\Delta\overrightarrow{g_j}(\vec{r})\cdot\vec{r}$ where $\Delta\overrightarrow{g_j}$ represent the variation of the crystalline vector compared to its unstrained state.

$$\begin{aligned} \forall(x,y)\in\mathbb{R}^2, I_C(\vec{r}) &= \sum_{j=-\infty}^{j=+\infty} C_j(\vec{r})e^{i(\vec{g_j}\cdot\vec{r})} \\ \forall(x,y)\in\mathbb{R}^2, I_C(\vec{r}) &= \sum_{j=-\infty}^{j=+\infty} A_j e^{i(\vec{g_j}\cdot\vec{r})+iP_{g_j}(\vec{r})} \end{aligned} \tag{7}$$

By applying GPA (T 2) on eq. (7), $P_{g_j}(\vec{r})$ can be extracted. Then by applying A 4, the gradient ∇ of $P_{g_j}(\vec{r})$ can be approximate as follows

$$\nabla P_{g_j}(\vec{r}) = 2\pi[\nabla(\Delta\overrightarrow{g_j}\cdot\vec{r})] \approx 2\pi\Delta\overrightarrow{g_j(\vec{r})} \tag{8}$$

⋆ Source: [?]

⋆ Ref by: T 2, IM 3, IM 5

3.2.4 Instance Models

IM 1 **Calculate the crystal reflections in 3D**

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

IM 2 **Project the crystal reflections in sampling base**

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