

Software Requirements Specifications (SRS)

STEM Moiré GPA

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September 24, 2017

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Table 1: **Revision History**

Date	Version	Notes
19/09/2017	1.0	First Draft

1 Reference Material

1.1 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
s	time	second

1.2 Table of Symbols

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

Symbol	Unit	Description
δ		Dirac delta function
ε		Strain tensor
\mathcal{FT}		Fourier transform
$\overrightarrow{g_{hkl}}$	nm ⁻¹	[hkl] crystalline wave vector
i		Imaginary unit
\mathbb{N}		Set of natural numbers
ω		Rotation tensor
p	nm	pixel size
\mathbb{R}		Set of real numbers
\mathbb{Z}		Set of integer numbers

1.3 Abbreviations and Acronyms

symbol	description
A	Assumption
DC	Data Constraint
DD	Data Definition
EM	Electron Micrograph
GD	General Definition
GPA	Geometrical Phase Analysis
GS	Goal Statement
I	Intensity (or number of counts
IM	Instance Model
LC	Likely Change
PS	Physical System Description
R	Requirement
SMH	STEM Moiré Hologram
SRS	Software Requirements Specification
STEM	Scanning Transmission Electron Microscopy
T	Theoretical Model

2 Introduction

2.1 Purpose of Document

2.2 Scope of Requirements

2.3 Characteristics of Intended Reader

2.4 Organization of Document

3 General System Description

This section identifies the interfaces between the system and its environment, describes the user characteristics and lists the system constraints.

3.1 System Context

- User Responsibilities:
 -
- STEM Moiré GPA Responsibilities:
 - Detect data type mismatch, such as a string of characters instead of a floating point number
 -

3.2 User Characteristics

The end user of STEM Moiré GPA should have an understanding of undergraduate Level 1 Calculus and Physics.

3.3 System Constraints

4 Specific System Description

4.1 Problem Description

STEM Moiré GPA project is software capable of converting a STEM Moiré hologram into 2D strain maps.

4.1.1 Terminology and Definitions

Regarding the complexity of the electron/matter interaction, some crude simplifications are proposed to describe the terminologies below. While sometimes not realistic, the simplifications are here to help in visualizing the context and the type of data the STEM Moiré GPA software is subjected to. Nevertheless, all the simplifications are not affecting the definition of the concept used at the software level.

- **2D Cartesian coordinate system:** orthonormal coordinate system model by the orthonormal base $\mathcal{B} = (O, \vec{u}_x, \vec{u}_y)$ such that any vector \vec{r} can be expressed as the following:

$$\forall (x, y) \in \mathbb{R}^2, \vec{r} = x\vec{u}_x + y\vec{u}_y \quad (1)$$

- **Pixel:** smallest addressable element sampling a 2D continuum.
- **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 fig. 1. The positions of the STEM probe are located at the intersection of the black grid lines.

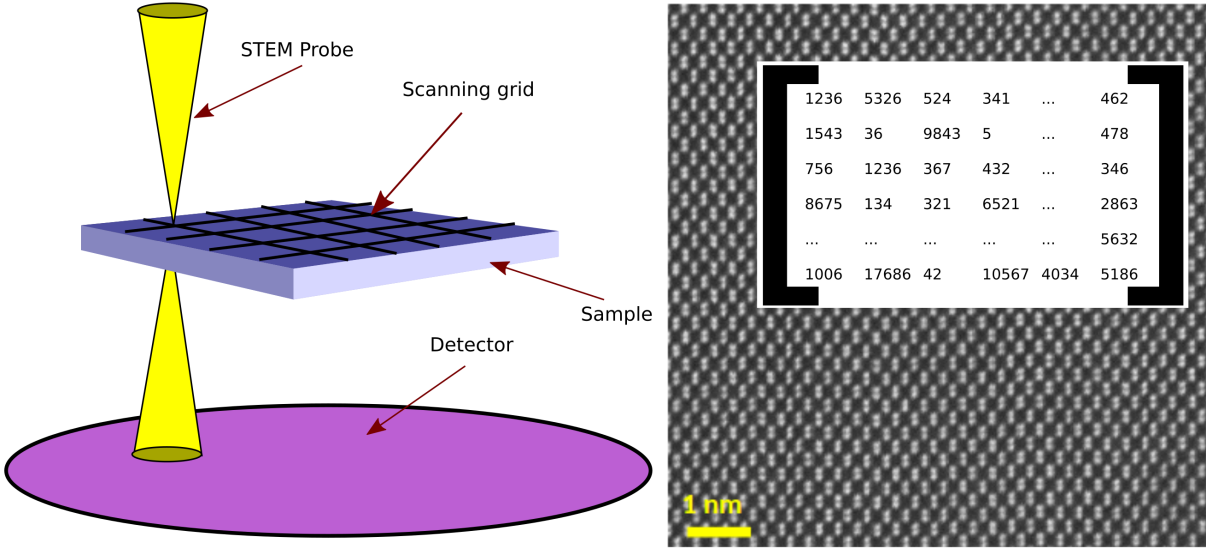


Figure 1: On the left hand side, a schematic of the STEM EM formation with the STEM probe scanning the sample at each intersection of the grid lines. The electrons crossing the sample are collected on the detector and counted during the acquisition time. On the right hand side is presented a STEM EM on a pure silicon sample revealing its atomic structure. In the inset is highlighted the type of data the STEM EM corresponds to which is a 2D array.

- **Hologram**: Result from an interference between two or multiples waves.
- **Moiré hologram**: Result from interference between two or multiple waves with similar but not equal wave numbers (or wave vectors in 2D).
- **Crystal lattice**: Arrangement of atoms forming matter.
- **STEM Moiré hologram (SMH)**: EM collected in STEM and resulting from the Moiré interference between the scanning grid and the crystal lattice.
- **Strain map**: 2D array mapping the evolution of one element of the 2D strain or rotation tensor.

4.1.2 Physical System Description

The physical system of STEM Moiré GPA, as shown in Figure ?, includes the following elements:

4.1.3 Goal Statements

Given the system description, the goal statements are:

GS 1 Extract quantitatively the chosen crystalline wave vectors. This corresponds to extract \vec{g}_j from I_{SMH} .

GS 2 Extract quantitatively the variation of the chosen crystalline wave vectors. This corresponds to extract P_{g_j} from I_{SMH} .

GS 3 Display, on each pixel, all the elements of the 2D strain and rotation tensor which are the parameters ε_{xx} , ε_{xy} , ε_{yy} and ω_{xy} in eq. (7)

4.2 Solution Characteristics Specification

4.2.1 Assumptions

A 1 The microscope has a limit of resolution corresponding to the probe size and thus cannot resolve any spatial frequency higher than g_{jim} .

A 2 Since the STEM EM is discretized in pixels, the smallest features possible is composed of two pixels. Therefore, in reciprocal space, the maximum range of spatial frequency detectable is $\Gamma = [-\frac{1}{2p}, \frac{1}{2p}]^2$.

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).

A 4 The variation of the strain field (or deformation field) is small.

A 5 The strain magnitude is small (elastic regime). As a consequence, $\frac{\|\tilde{\Delta g}\|}{\|\vec{g}\|} < 0.1$

A 6 The user knows the crystal structure of the sample analysed at its unstrained state or can provide a reference in which is embedded the crystal structure information at its unstrained state.

4.2.2 Theoretical Models

T 1 Sampling

- Equation: Equation (3)
- Description: In the 2D Cartesian coordinate system, the scanning grid can be seen as sampler S of continuous function f . For the purpose of the STEM Moiré GPA, 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:

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

For shorter notations, it is position 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)

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

- Source: Trouver un truc pr sampling (bouquin sur la table d'isobel)
- Ref by:

T 2 Geometrical Phase Analysis

- Equation: Equation (6)
- Description: Let consider a function f decomposed in Fourier series as the following with

$$\begin{aligned} \forall \vec{r} = (x_1, \dots, x_n) \in \mathbb{R}^n, f(\vec{r}) &= \sum_{j=-\infty}^{j=+\infty} C_j e^{i(\vec{k}_j \cdot \vec{r})} \\ \forall \vec{r} = (x_1, \dots, x_n) \in \mathbb{R}^n, f(\vec{r}) &= \sum_{j=-\infty}^{j=+\infty} A_j e^{i((\vec{k}_j \cdot \vec{r}) + B_j)} \end{aligned} \quad (4)$$

The objective of GPA is to extract one chosen B_j from f in Fourier space. Let's consider the Fourier transform of f such that

$$\begin{aligned} \forall \vec{\nu} = (\nu_1, \dots, \nu_n) \in \mathbb{R}^n, \forall \vec{r} = (x_1, \dots, x_n) \in \mathbb{R}^n, \tilde{f}(\vec{\nu}) &= \mathcal{FT}(f(\vec{r})) \\ \forall \vec{\nu} \in \mathbb{R}^n, \tilde{f}(\vec{\nu}) &= \sum_{j=-\infty}^{j=+\infty} A_j e^{iB_j} \delta(\vec{k}_j - \vec{\nu}) \end{aligned} \quad (5)$$

If all the \vec{k}_j are separated enough to be isolated with a mask, then B_j can be extracted by considering the inverse Fourier transform of the masked area and expressing the result in term of amplitude and phase. In mathematical formalism, B_j is extracted as follows.

$$\begin{aligned} \text{if } \exists M : \begin{cases} \mathbb{R} \longrightarrow \mathbb{C} \\ \vec{\nu} \longmapsto M(\vec{\nu}) \end{cases} / \begin{cases} M(\vec{\nu}) \tilde{f}(\vec{\nu}) = A_j e^{iB_j} & \text{for } \vec{\nu} \in [(\nu_1^D, \dots, \nu_n^D), (\nu_1^U, \dots, \nu_n^U)] \\ M(\vec{\nu}) \tilde{f}(\vec{\nu}) = 0 \end{cases} \\ \Rightarrow \begin{aligned} |\mathcal{FT}^{-1}(M(\vec{\nu}) \tilde{f}(\vec{\nu}))(\vec{r})| &= A_j \\ \arg(\mathcal{FT}^{-1}(M(\vec{\nu}) \tilde{f}(\vec{\nu}))(\vec{r})) &= B_j \end{aligned} \end{aligned} \quad (6)$$

- Source:
- Ref by:

Description of the GPA method in a 1D cartesian coordinate system

Let's consider a function f such that

$$\forall x \in \mathbb{R}, f(x) = C_0 e^{i(k_0 x)} + C_1 e^{i(k_1 x)}$$

Applying the GPA method on f ,

$$\forall \nu \in \mathbb{R}, \forall x \in \mathbb{R}, \widetilde{f(\nu)} = C_0 \delta(k_0 - \nu) + C_1 \delta(k_1 - \nu)$$

T 3 Strain Model

- Equation: Equation (7)
- Description: In infinitesimal strain theory with small displacement and small gradient of displacement, the displacement gradient tensor ∇u can be decomposed in two independent tensors: the symmetric strain tensor ε and the anti-symmetric rotation tensor ω . Their relationship can be described as follows:

$$\begin{aligned} \nabla u &= \varepsilon + \omega = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} \\ \varepsilon_{xy} & \varepsilon_{yy} \end{bmatrix} + \begin{bmatrix} 0 & \omega_{xy} \\ -\omega_{xy} & 0 \end{bmatrix} \\ \varepsilon &= \frac{1}{2}(\nabla u + (\nabla u)^T) \\ \omega &= \frac{1}{2}(\nabla u - (\nabla u)^T) \end{aligned} \tag{7}$$

- Source:
- Ref by:

T 4 Interferometry

- Equation: Equation (9)
- Description: Let consider two monochromatic plane waves ψ_1 and ψ_2 with their respective amplitude A_j , phase ϕ_j and wave vector \vec{k}_j in the 2D Cartesian system interfering with each other. The resulting hologram ψ_H represented by the intensity I_H can be modelled as follows with :

$$\forall (x, y) \in \mathbb{R}^2, \psi_H(\vec{r}) = \psi_1 + \psi_2 = A_1 e^{i(\vec{k}_1 \cdot \vec{r}) + i\phi_1} + A_2 e^{i(\vec{k}_2 \cdot \vec{r}) + i\phi_2} \tag{8}$$

$$\forall(x, y) \in \mathbb{R}^2, I_H(\vec{r}) = \psi_H \psi_H^* = A_1^2 + A_2^2 + A_1 A_2 (e^{i(\vec{k}_1 - \vec{k}_2) \cdot \vec{r} + i(\phi_1 - \phi_2)} + e^{i(\vec{k}_2 - \vec{k}_1) \cdot \vec{r} + i(\phi_2 - \phi_1)}) \quad (9)$$

The more waves are contributing to the hologram, the more complex eq. (9) will be. However, similar factors will appear with constants and cross product terms.

- Source:
- Ref by:

4.2.3 General Definitions

GD 1 Strain in crystal lattice

- Equation: Equation (12)
- 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.

$$\forall(x, y) \in \mathbb{R}^2, I_C(\vec{r}) = \sum_{j=-\infty}^{j=+\infty} C_j e^{i(\vec{g}_j \cdot \vec{r})} \quad (10)$$

If the crystal is elastically 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. (10). 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 $P_{g_j}(\vec{r}) = 2\pi \Delta \vec{g}_j(\vec{r}) \cdot \vec{r}$ where $\Delta \vec{g}_j$ represent the variation of the crystalline vector compared to its unstrained state.

$$\begin{aligned} \forall(x, y) \in \mathbb{R}^2, I_C(\vec{r}) &= \sum_{j=-\infty}^{j=+\infty} C_j(\vec{r}) e^{i(\vec{g}_j \cdot \vec{r})} \\ \forall(x, y) \in \mathbb{R}^2, I_C(\vec{r}) &= \sum_{j=-\infty}^{j=+\infty} A_j e^{i(\vec{g}_j \cdot \vec{r}) + i P_{g_j}(\vec{r})} \end{aligned} \quad (11)$$

Applying GPA (T 2) on eq. (11), $P_{g_j}(\vec{r})$ can be extracted. Applying A 4, the gradient ∇ of $P_{g_j}(\vec{r})$ can be approximate as follows

$$\nabla P_{g_j}(\vec{r}) = 2\pi [\nabla(\Delta \vec{g}_j(\vec{r}))]^T \vec{r} + 2\pi \Delta \vec{g}_j(\vec{r}) \approx 2\pi \Delta \vec{g}_j(\vec{r}) \quad (12)$$

- Source: Ref Hytch1998

- Ref by:

GD 2 STEM Moiré hologram

- Equation: Equation (15)
- Description: Combining eq. (11) and eq. (2), a STEM Moiré hologram I_{SMH} can be described as follows

$$\forall (x, y) \in \mathbb{R}^2, I_{SMH}(\vec{r}) = \sum_{q \in Q} \delta(\vec{r} - p\vec{q}) \times \sum_{j=-\infty}^{j=+\infty} A_j e^{i(\vec{g}_j \cdot \vec{r}) + iP_{g_j}(\vec{r})} \quad (13)$$

By modifying p the scanning periodicity (or the pixel size), it is possible to adjust the spatial frequency of the SMH solving eq. (13). Applying A 1, the expression of I_C in eq. (11) is simplified since the series becomes a finite sum.

$$\forall (x, y) \in \mathbb{R}^2, I_C(\vec{r}) = \sum_{j=-j_{lim}}^{j=+j_{lim}} A_j e^{i(\vec{g}_j \cdot \vec{r}) + iP_{g_j}(\vec{r})} \quad (14)$$

Therefore, the STEM Moiré hologram I_{SMH} is also simplified as follows:

$$\forall (x, y) \in \mathbb{R}^2, I_{SMH}(\vec{r}) = \sum_{q \in Q} \delta(\vec{r} - p\vec{q}) \times \sum_{j=-j_{lim}}^{j=+j_{lim}} A_j e^{i(\vec{g}_j \cdot \vec{r}) + iP_{g_j}(\vec{r})} \quad (15)$$

- Source:
- Ref by:

From sampling to a hologram

Since the Dirac comb function is also periodic, the sampler can also be represented into Fourier series

$$\forall (x, y) \in \mathbb{R}^2, S(\vec{r}) = \sum_{q \in Q} \delta(\vec{r} - p\vec{q}) = \frac{1}{(2\pi)^2} \sum_{q \in Q} \sum_{l=-\infty}^{l=+\infty} e^{il(\vec{r} - p\vec{q})} \quad (16)$$

Using eq. (16) in eq. (15), it is possible to recognize an interference equation between multiple plane waves (a more complex version of eq. (9)).

$$I_{SMH}(\vec{r}) = \frac{1}{(2\pi)^2} \sum_{q \in Q} \sum_{l=-\infty}^{l=+\infty} \sum_{j=-j_{lim}}^{j=+j_{lim}} A_j e^{i(\vec{g}_j \cdot \vec{r} + l(\vec{r} - p\vec{q})) + iP_{g_j}(\vec{r})} \quad (17)$$

GD 3 Deformation gradient tensor

Equation: Equation (18)

Description: If $\vec{g}_j = g_{j_x} \vec{u}_x + g_{j_y} \vec{u}_y$ and $\Delta \vec{g}_j = \Delta g_{j_x} \vec{u}_x + \Delta g_{j_y} \vec{u}_y$ are known in the base \mathcal{B} for two non-collinear crystalline wave vectors, then the strain deformation tensor can be deduced by calculating first both the unstrained matrix G and the variation of the crystalline wave vectors matrix ΔG . Then the deformation gradient tensor ∇u is estimated as the following with I_d representing the identity matrix (see annexe D in refHytch1998 and equation (30) in refRouviere2005).

$$\begin{aligned} G_{ref} &= \begin{bmatrix} g_{1x} & g_{1y} \\ g_{2x} & g_{2y} \end{bmatrix} \\ \Delta G &= \begin{bmatrix} \Delta g_{1x} & \Delta g_{1y} \\ \Delta g_{2x} & \Delta g_{2y} \end{bmatrix} \\ \nabla u &= (\Delta G^T)^{-1} G_{ref}^T - I_d \end{aligned} \tag{18}$$

Source:

Ref by:

4.2.4 Data Definitions

DD 1 STEM Moiré hologram

- Equation: eq. (7)
- Description:
- Source:
- Ref by:

DD 2 Crystal structure reference

- Equation:
- Description:
- Source:
- Ref by:

DD 3 Moiré wave vector

- Equation:
- Description:

- Source:
- Ref by:

DD 4 Crystalline wave vector

- Equation:
- Description:
- Source:
- Ref by:

DD 5 Sampling vector operating in Γ frequency range

- Equation: $\vec{g}_j^C = \vec{g}_j^M + \frac{1}{p}\vec{q}_j^C$
- Description:
- Source:
- Ref by:

DD 6 Mask M isolating a spatial frequency

- Equation:
- Description:
- Source:
- Ref by:

4.2.5 Instance Models

IM 1 Simulate the SMH on a reference to determine \vec{q}_j^C for each \vec{g}_j^M

- Input: I_{ref}, p
- Output: $I_{sim}, (n_j; m_j), \vec{g}_j^M$
- Source:
- Ref by:

Derivation of IM 1

IM 2 Convert the Moiré geometric phase into Crystalline geometric phase

- Input: $I_{SMH}, M, \vec{q}_j, \Delta \vec{g}_j^M$
- Output: $\Delta \vec{g}_j^C$
- Source:
- Ref by:

IM 3 Strain calculation using 2 non-crystalline wave vectors

- Input: $g_{1x}^C, g_{1y}^C, g_{2x}^C, g_{2y}^C, \Delta g_{1x}^C, \Delta g_{1y}^C, \Delta g_{2x}^C, \Delta g_{2y}^C$
- Output: $\varepsilon_{xx}, \varepsilon_{xy}, \varepsilon_{yy}, \omega_{xy}$
- Source:
- Ref by:

Derivation of ...

4.2.6 Data Constraints

4.2.7 Properties of a Correct Solution

A correct solution must exhibit

5 Requirements

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

5.1 Functional Requirements

5.2 Nonfunctional Requirements

6 Likely Changes

7 Traceability Matrices and Graphs

8 Appendix

8.1 Symbolic Parameters