Software Requirements Specifications (SRS)
STEM Moiré GPA

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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. The symbols are listed in alphabetical order.

Symbol	**Unit**	**Description**
A_C	m^2	coil surface area
A_{in}	m^2	surface area over which heat is transferred in

1.3 Abbreviations and Acronyms

symbol	description
A	Assumption
DD	Data Definition
EM	Electron Micrograph
GD	General Definition
GPA	Geometrical Phase Analysis
GS	Goal Statement
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
STEM Moiré GPA	
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 with $\mathbb{R}$ representing the set of real space:

$$\forall (x, y) \in \mathbb{R}^2, \vec{r} = x\vec{u_x} + y\vec{u_y} \tag{1}$$

- **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.

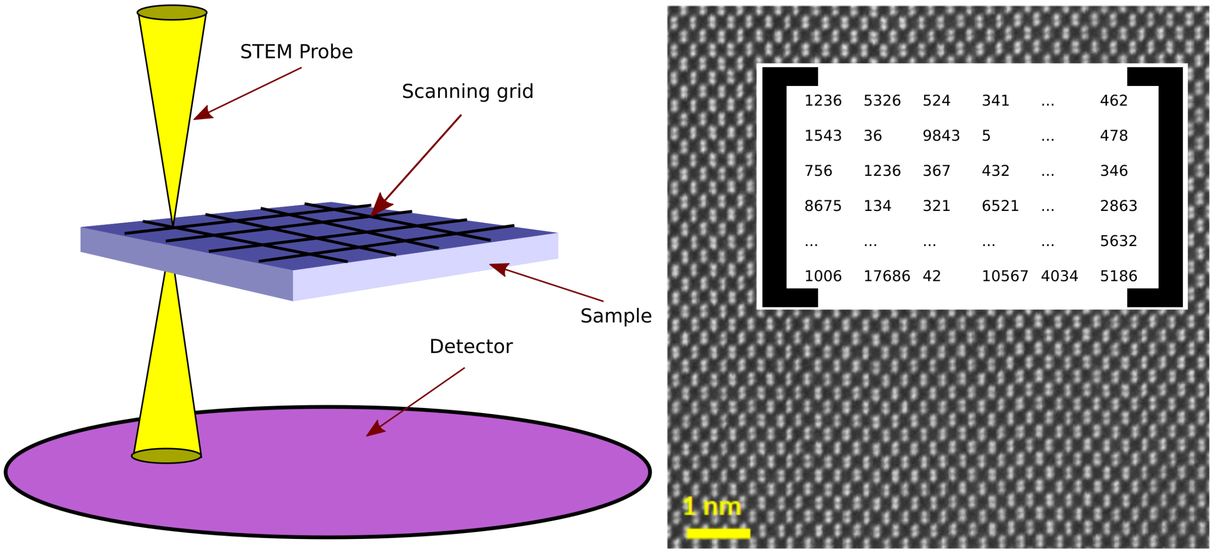

Figure 1: On the left hand side, a schematic of the STEM EM formation with the STEM probe scanning the sample at each intersection of the grid lines. The electrons crossing the sample are collected on the detector and counted during the acquisition time. On the right hand side is presented a STEM EM 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.

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 functio

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

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

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

- **Hologram**: Result from an interference between two or multiples waves.
  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. The hologram ψ_H and the

resulting intensity from the hologram I_H can be modelled as follows with i representing the imaginary unit:

$$\forall(x,y)\in\mathbb{R}^2, \psi_H(\vec{r}) = \psi_1+\psi_2 = A_1 e^{i(\vec{k_1}\cdot\vec{r})+i\phi_1} + A_2 e^{i(\vec{k_2}\cdot\vec{r})+i\phi_2}$$
$$\forall(x,y)\in\mathbb{R}^2, I_H(\vec{r}) = \psi_H\psi_H^* = A_1^2+A_2^2+A_1A_1(e^{i(\vec{k_1}-\vec{k_2})\cdot\vec{r}+i(\phi_1-\phi_2)} + e^{i(\vec{k_2}-\vec{k_1})\cdot\vec{r}+i(\phi_2-\phi_1)}) \tag{4}$$

The more waves are contributing to the hologram, the more complex eq. (4) will be. However, similar factors will appear with constants and cross product terms.

- **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.
  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.

$$\forall(x,y)\in\mathbb{R}^2, I_C(\vec{r}) = \sum_{j=-\infty}^{j=+\infty} C_j e^{i(\vec{g_j}\cdot\vec{r})} \tag{5}$$

  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. (5). 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 (ref hytch 1998).

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

- **STEM Moiré hologram (SMH)**: EM collected in STEM and resulting from the Moiré interference between the scanning grid and the crystal lattice.

  Combining eq. (6) and eq. (2), a STEM Moiré hologram I_{SMH} can be described as follows

$$I_{SMH}(\vec{r}) = \sum_{q\in Q}\delta(\vec{r}-p\vec{q}) \times \sum_{j=-\infty}^{j=+\infty} A_j e^{i(\vec{g_j}\cdot\vec{r})+iP_{g_j}(\vec{r})} \tag{7}$$

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

$$\forall(x,y) \in \mathbb{R}^2, S(\vec{r}) = \sum_{q \in Q} \delta(\vec{r} - p\vec{q}) = \frac{1}{(2\pi)^2} \sum_{q \in Q} \sum_{l=-\infty}^{l=+\infty} e^{il(\vec{r}-p\vec{q})} \tag{8}$$

Using eq. (8) in eq. (7), it is possible to recognize an interference equation between multiple plane waves (a more complex version of eq. (4).

$$I_{SMH}(\vec{r}) = \frac{1}{(2\pi)^2} \sum_{q \in Q} \sum_{l=-\infty}^{l=+\infty} \sum_{j=-\infty}^{j=+\infty} A_j e^{i(\vec{g_j}\cdot\vec{r}+l(\vec{r}-p\vec{q}))+iP_{g_j}(\vec{r})} \tag{9}$$

By modifying p the scanning periodicity (or the pixel size), it is possible to adjust the spatial frequency of the SMH solving eq. (9)

- **Strain map**: 2D array mapping the evolution of one element of the 2D strain or rotation tensor.
  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 for two non-collinear crystalline wave vectors, then the strain tensor can be deduced. First both the unstrained matrix G and the variation of the crystalline wave vectors matrix ΔG are generated to calculate the distortion matrix D with I_d representing the identity matrix.

$$\begin{gathered} G_{ref} = \begin{bmatrix} g_{1_x} & g_{1_y} \\ g_{2_x} & g_{2_y} \end{bmatrix} \\ \Delta G = \begin{bmatrix} \Delta g_{1_x} & \Delta g_{1_y} \\ \Delta g_{2_x} & \Delta g_{2_y} \end{bmatrix} \\ D = (\Delta G^T)^{-1} {G_{ref}}^T - I_d \end{gathered} \tag{10}$$

  From the distortion matrix, the strain and rotation tensor can be finally evaluated with ε the strain tensor and ω the rotation tensor (see annexe D in refHytch1998 and equation (30) in refRouviere2005).

$$\begin{gathered} \varepsilon = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} \\ \varepsilon_{xy} & \varepsilon_{yy} \end{bmatrix} = \frac{1}{2}(D + D^T) \\ \omega = \begin{bmatrix} 0 & \omega_{xy} \\ -\omega_{xy} & 0 \end{bmatrix} = \frac{1}{2}(D - D^T) \end{gathered} \tag{11}$$

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. (11)

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_{lim}. As a consequence, the expression of I_C in eq. (6) is simplified since the series becomes a finite sum considering F a floor function.

$$\forall (x,y) \in \mathbb{R}^2, I_C(\vec{r}) = \sum_{j=-F(g_{lim})}^{j=+F(g_{lim})+1} A_j e^{i(\vec{g_j}\cdot\vec{r})+iP_{g_j}(\vec{r})} \tag{12}$$

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 $[-\frac{1}{2p}, \frac{1}{2p}]^2$.

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. As a consequence $\nabla(\Delta\overrightarrow{g(\vec{r})}\cdot\vec{r}) \approx \Delta\overrightarrow{g(\vec{r})}$

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

4.2.2 Theoretical Models

dwdqwd

4.2.3 General Definitions

Detailed derivation of simplified rate of change of temperature

4.2.4 Data Definitions

4.2.5 Instance Models

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