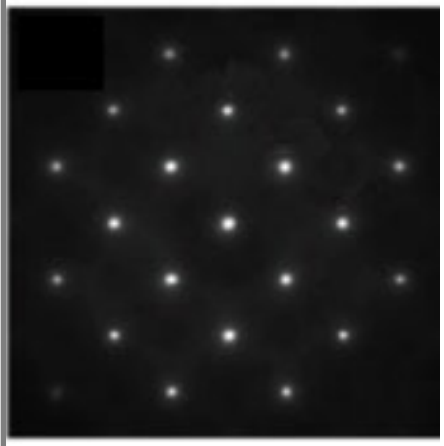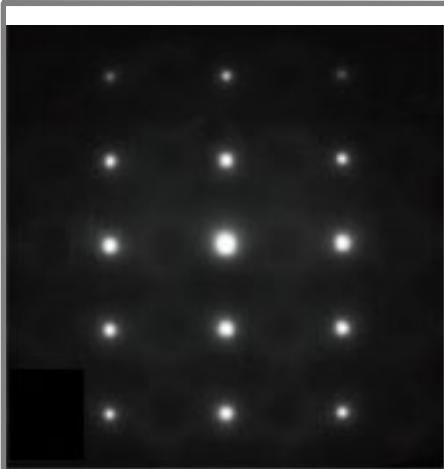# AI based material crystal structure analysis solution

LightVision Inc.
2023-06-21
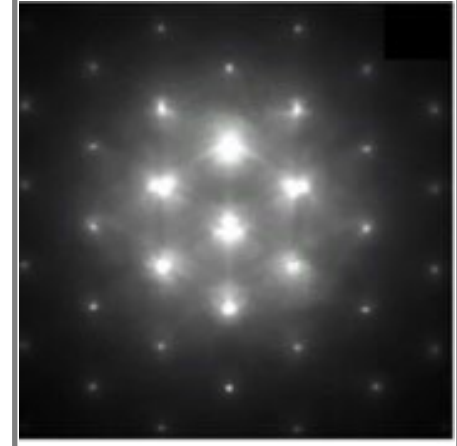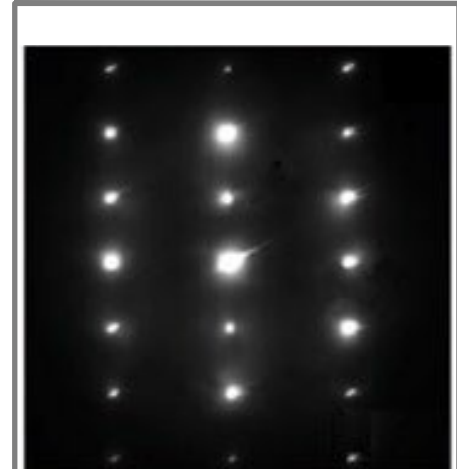
TEM Image Analysis

Analyzing 2D patterns in TEM(Transmission Electron Microscope) images to infer the 3D crystal structure of the material

AI based TEM SAED Pattern Analysis

[Existing TEM SAED pattern analysis method]
- Domain knowledge required
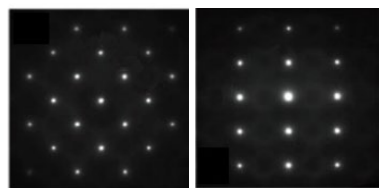- Take very long time to analyze the pattern
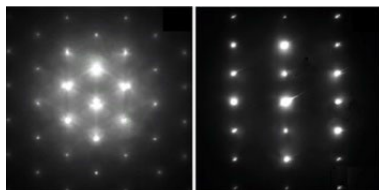
AI based TEM SAED analysis S/W

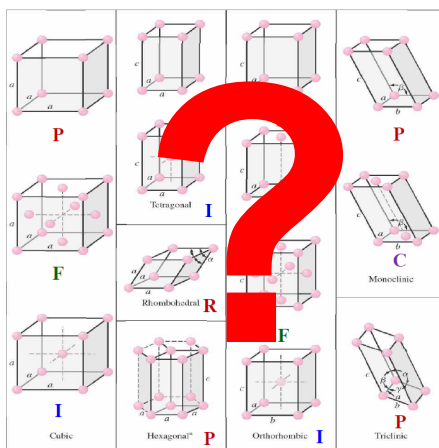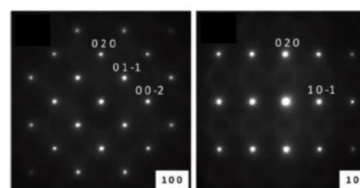**Crystal structure classification**

1st SAED pattern

VS
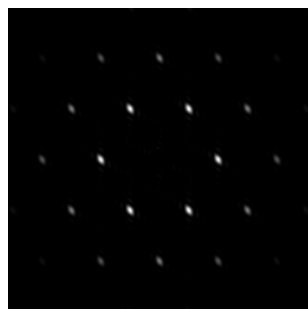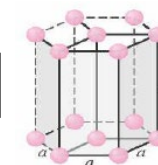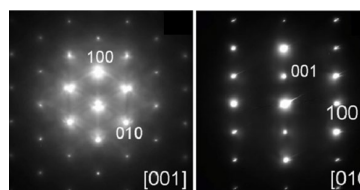
2nd SAED pattern

7 crystal systems / 14 crystal lattices

?

Body-Centered Cubic Structure
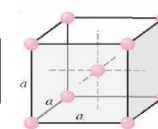
Hexagonal Structure

BiRh (SG: 194)

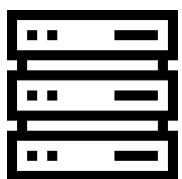C (SG: 227)

Pt (SG: 225)

He (SG: 229)

Real SEM/TEM Image Generation Technology

Golden Template based Defect Analysis

PROBLEM

Lack of data

Data imbalance
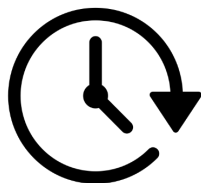
Time consuming
annotation task

SOLUTION

PatchMatch Algorithm

Synthetic non-defect images **(12,800)**

Real defect image **(250)**

Synthetic defect images **(12,800)**

Golden template generator

(a) input   (b) hole and guides   (c) completion result

(d) input   (e) hole   (f) completion (close up)

(g) same input   (h) hole and guides   (i) guided (close up)

(a) Initialization   (b) Propagation   (c) Search

[1] Barnes, Connelly, et al. "PatchMatch: A randomized correspondence algorithm for structural image editing." ACM Transactions on Graphics (ToG). Vol. 28. No. 3. ACM, 2009.

Defect Detection in SEM Image through AI Engine

Semiconductor defect detection in Scanning Electron Microscope (SEM) images
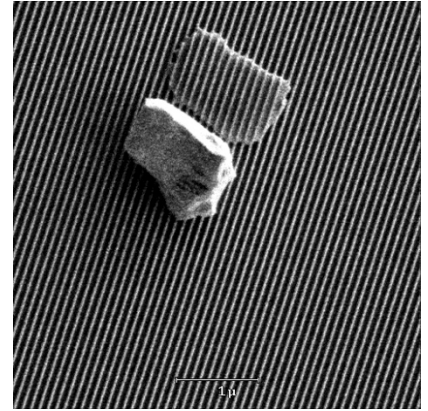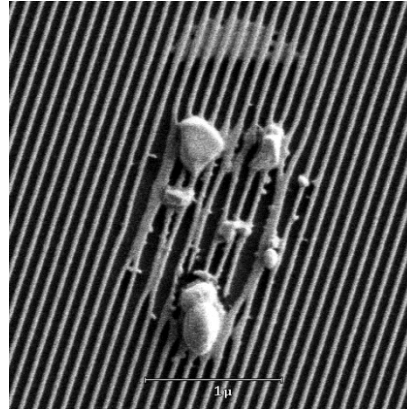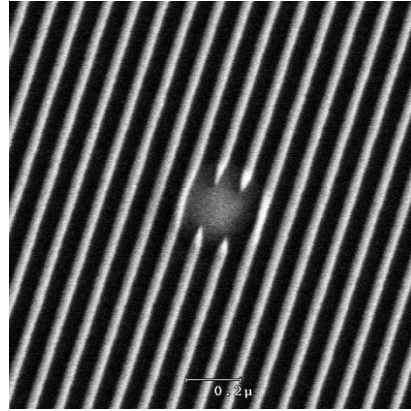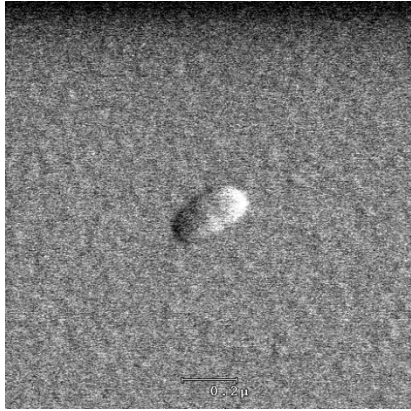
Detecting various type of defects through an AI engine

Right answer ⎯⎯⎯

Hypothesis ⎯⎯⎯

Detection result ⎯⎯⎯

Automatic analysis of TEM SADP

XTALAB

English | admin Founder

⊠ Crystal Structure Analysis ∨   ◎ Seismic Image Analysis ∨

Selected Area Diffraction Pattern Prec **Clear all TEM SADPs in the list**

≡ Clear All

Drop SADP images here or click to upload.

Drag & Drop zone for TEM SADP input

Ag4_[001]_171keV_20cm.png
8.5KB

✕

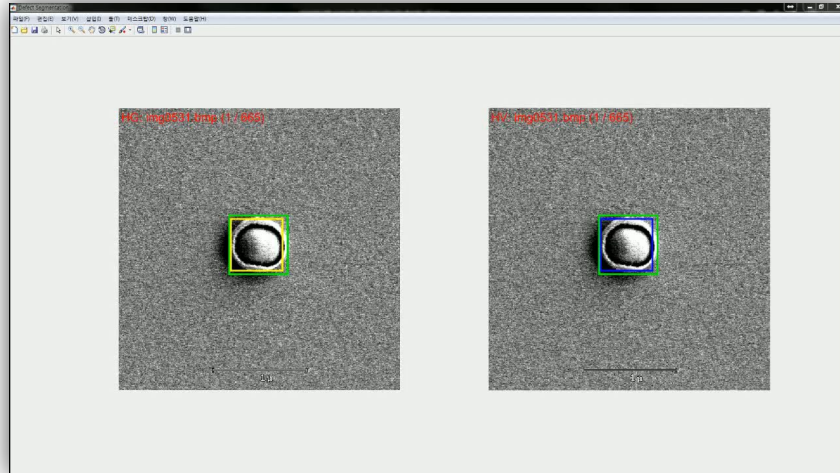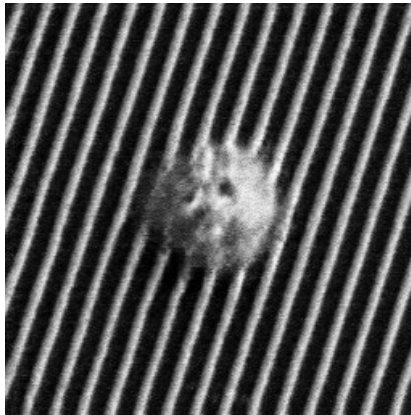**List of TEM SADPs**

Conventional Unit Cell | Display All

HM:P23 #195
a=14.775Å
b=14.775Å
c=14.775Å
α=90.000°
β=90.000°
γ=90.000°

Se1 #34

3D model of representative crystal structure of inferred space group (e.g., representative crystal structure of 195 space group)

SPACE GROUP PROBABILITY

195: 20%
206: 20%
225: 20%
227: 20%
229: 20%

0 10 20 30 40 50 60 70 80 90 100
■195 ■206 ■225 ■227 ■229

Display of space group inference probability (In case of non unique TEM SADP input, dispersed probability is displayed as a result)

POSSIBLE MATERIALS

$Na_8Al_6Si_6BrClO_{24}$ | $CeSe_2$ | SiO_2

Display list of possible materials belongs to the inferred space group

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Automatic analysis of TEM SADP

Clear all TEM SADPs in the list

Drag & Drop zone for TEM SADP input

Display of space group inference probability
(If unique TEM SADP is included, possible to infer space group at higher probability)

List of TEM SADPs
(possible to input more than 2 patterns)

3D model of representative crystal structure of inferred space group
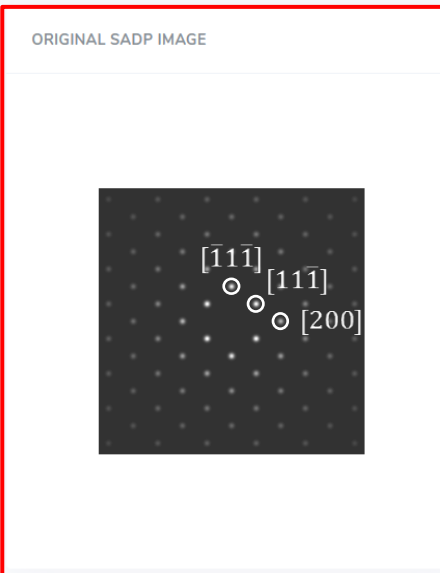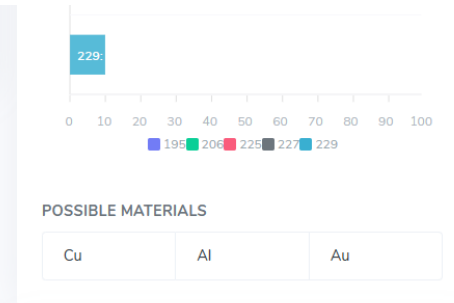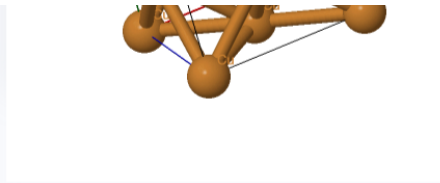**(e.g., representative crystal structure of 225 space group)**

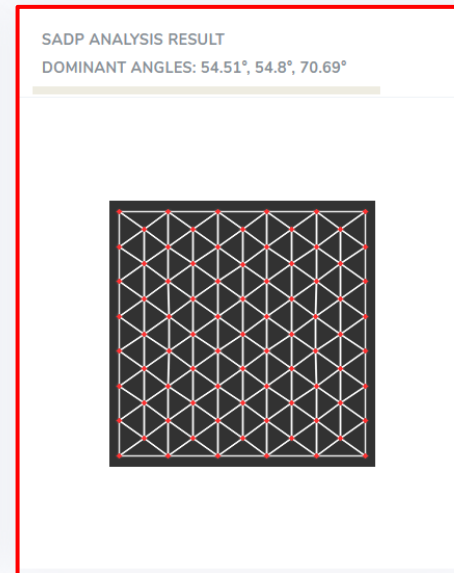**Display list of possible materials belongs to the inferred space group**

Thorough analysis of TEM SADP

**Click on TEM SAED pattern
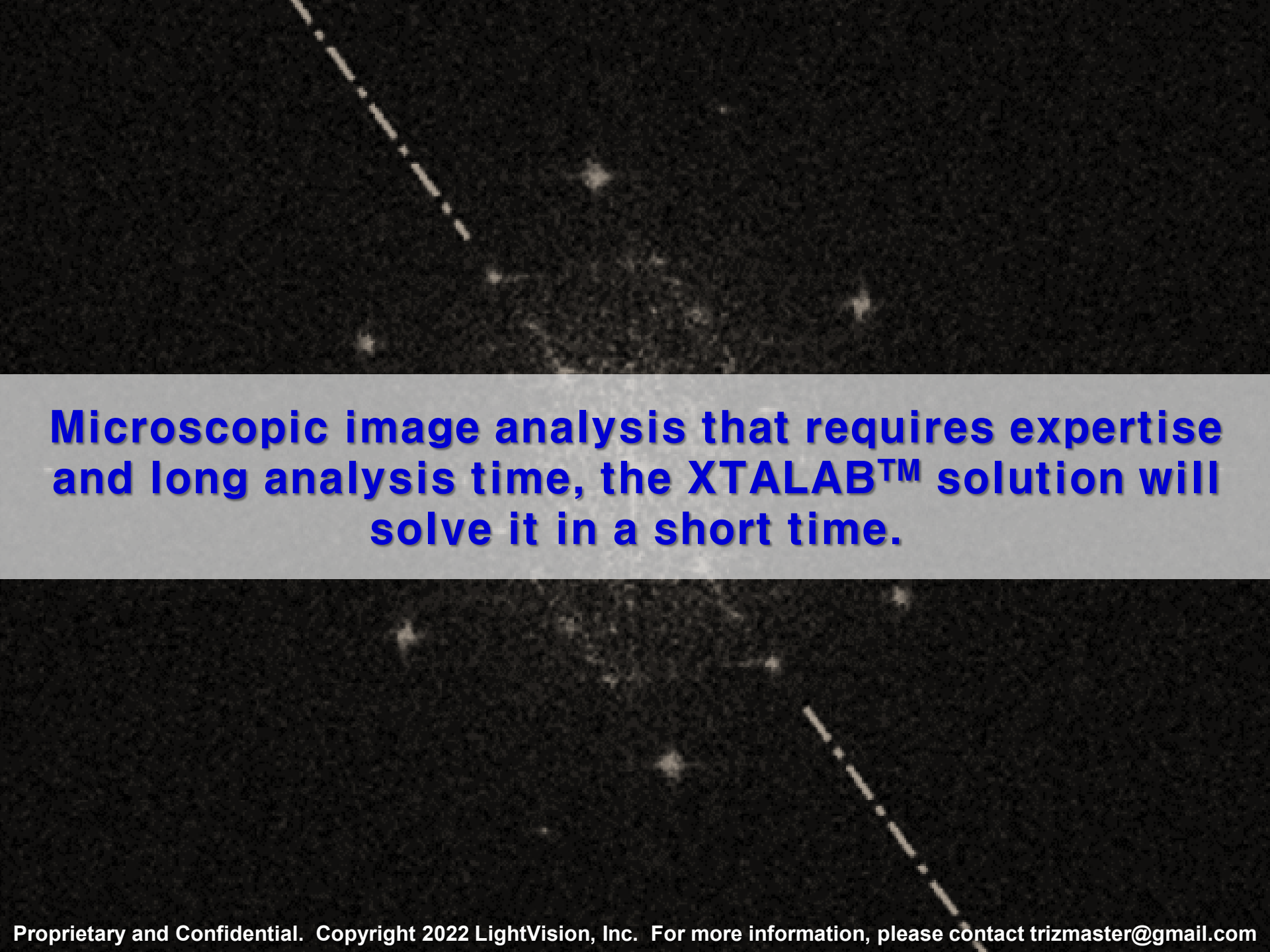if you want thorough analysis**

ORIGINAL SADP IMAGE

[$\overline{1}11$]

[111]

[200]

SADP ANALYSIS RESULT
DOMINANT ANGLES: 54.51°, 54.8°, 70.69°

POSSIBLE MATERIALS

| Cu | Al | Au |

229:

0 10 20 30 40 50 60 70 80 90 100

195 206 225 227 229

Ag4_[101]_238keV_30cm.png
11.8KB

**Display an original of
the analyzed TEM SAED pattern
(automatic indexing)**

**Display result of thorough analysis
(distances and angles between diffraction spots)**

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Microscopic image analysis that requires expertise and long analysis time, the XTALAB™ solution will solve it in a short time.