Ernst Ruska-Centrum für Mikroskopie und Spektroskopie mit Elektronen ER-C

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Differentiation of phases in phase change memory materials using 4D STEM

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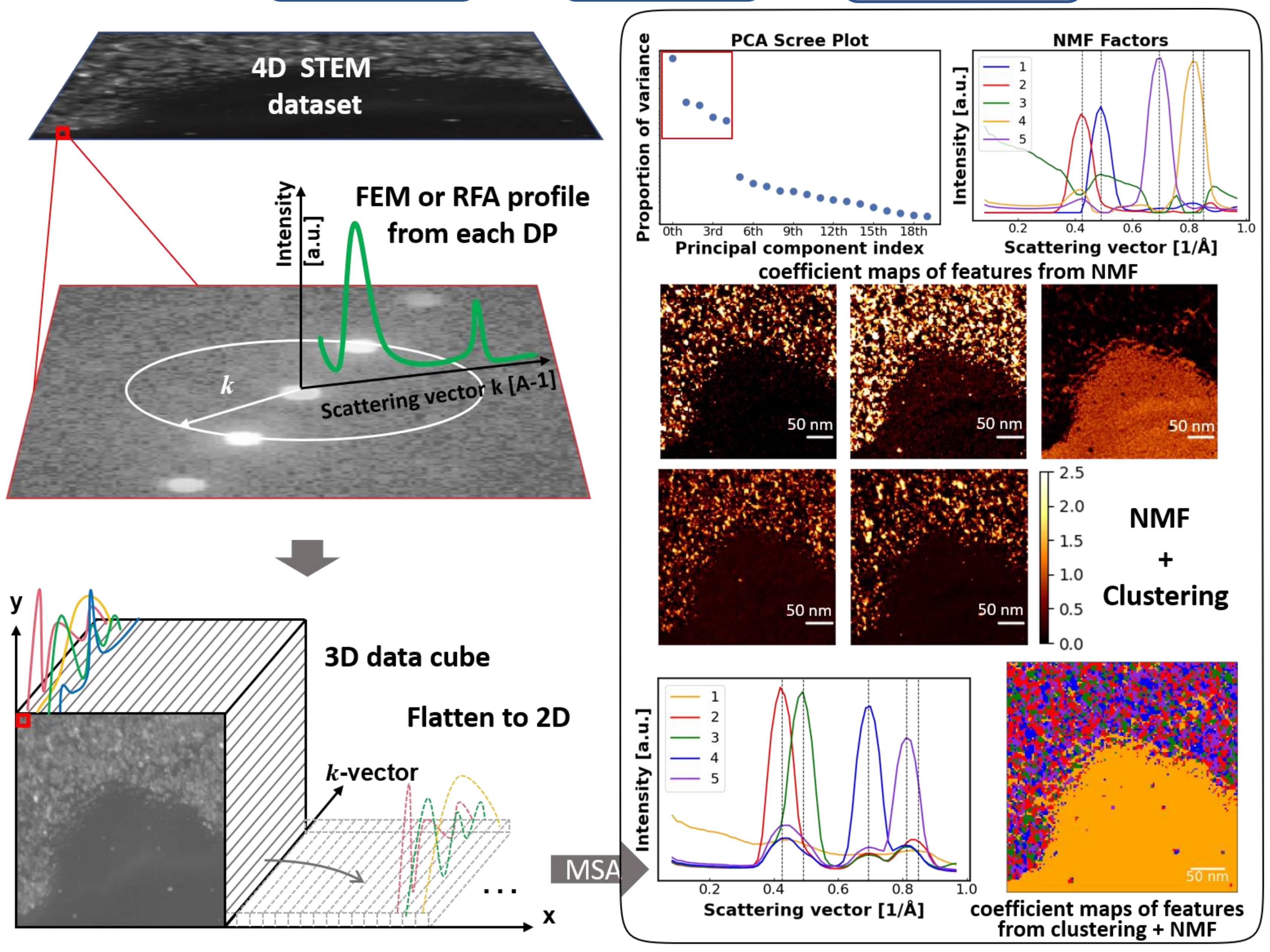
Introduction

With the rapid development of modern information technology, the novel approaches for storing and processing large volumes of data are being developed. Different electronic devices are under development. Phase change memories (PCM) that are based on chalcogenide materials are promising choices for data storage because phase transitions between amorphous and crystalline phases are quick and efficient. They are also promising for realizing multi-level storage. However, the resistance of the amorphous phase in a PCM cell can drift over time. It is important to determine the underlying mechanism of resistance drift and to develop methods that can be used to differentiate between local crystalline and amorphous phases efficiently. 4-dimensional scanning transmission electron microscopy (4D STEM) enables structural identification at nm resolution.[1] In this project, new analysis methods based on 4D STEM are applied to phase identification in phase change materials.

Methods

Diffraction patterns → Angular intensity → FEM RFA

→ 3D data cube → PCA NMF → Amorphous/ crystal map



FEM (Fluctuation electron microscopy)

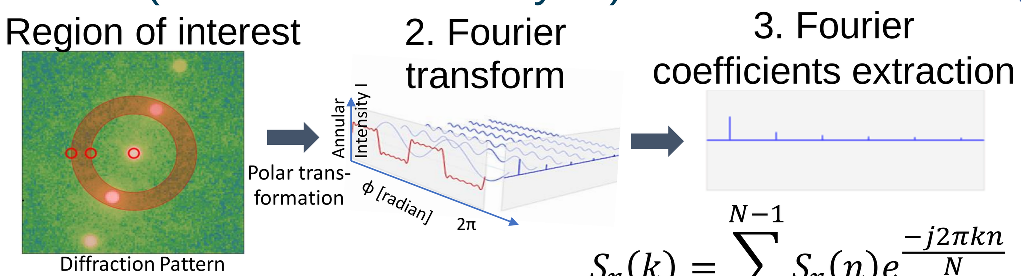
The normalized variance V of the intensity I from different positions on the specimen r.[2]

$$V(k,R) = \frac{\langle I(k,R,\mathbf{r})^2 \rangle_r}{\langle I(k,R,\mathbf{r}) \rangle_r^2} - 1$$

where <>r indicates averaging over r.

RFA (Radial Fourier analysis)

1. Region of interest 2. Fourier transform 3. Fourier coefficients extraction



Fourier coefficients Sr(k) are calculated.[3][4]

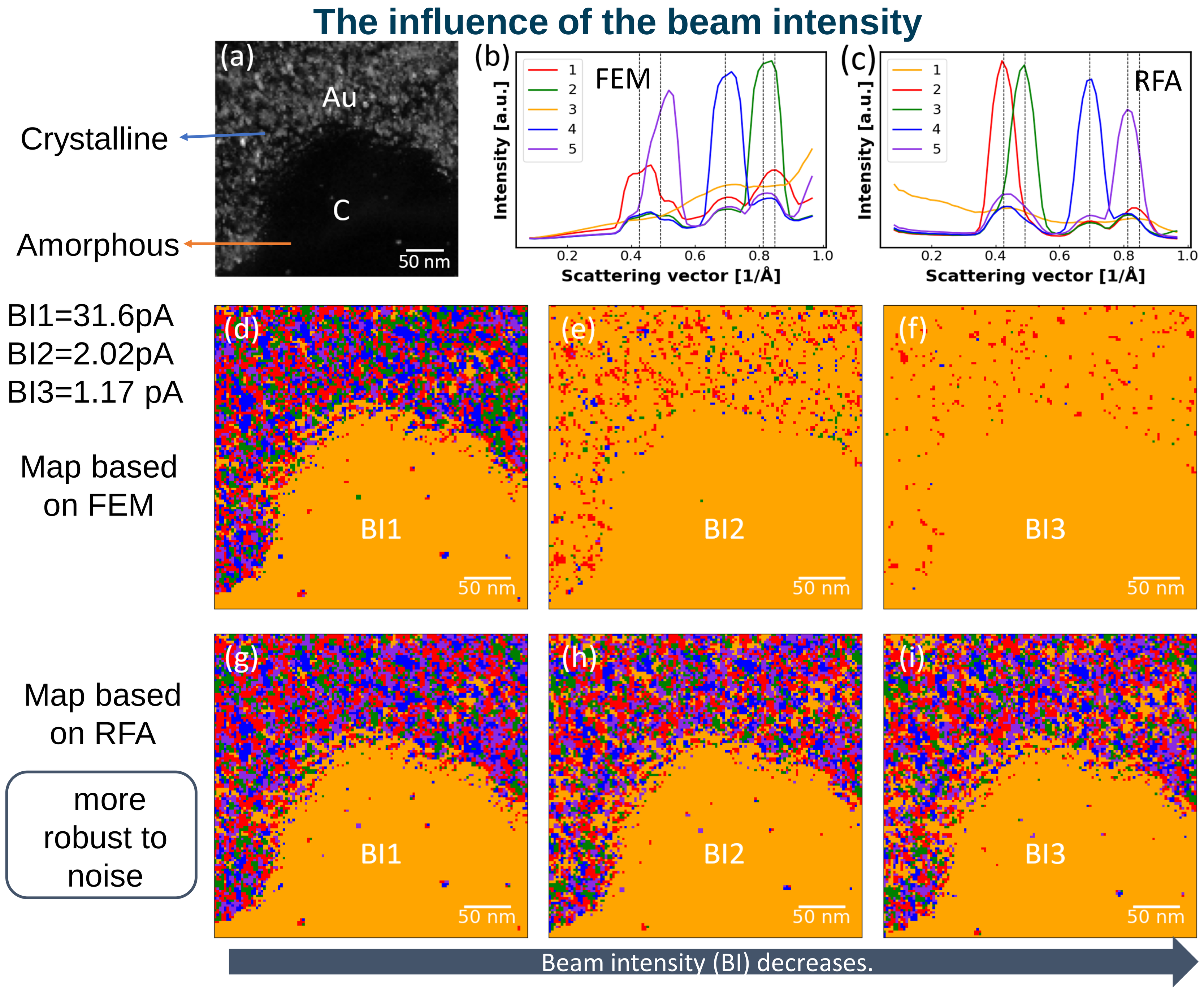
$$S_r(k) = \sum_{n=0}^{N-1} S_r(n) e^{\frac{-j2\pi kn}{N}}$$

$S_r(k)$ indicates k_{th} Fourier coefficient.

Experimental results

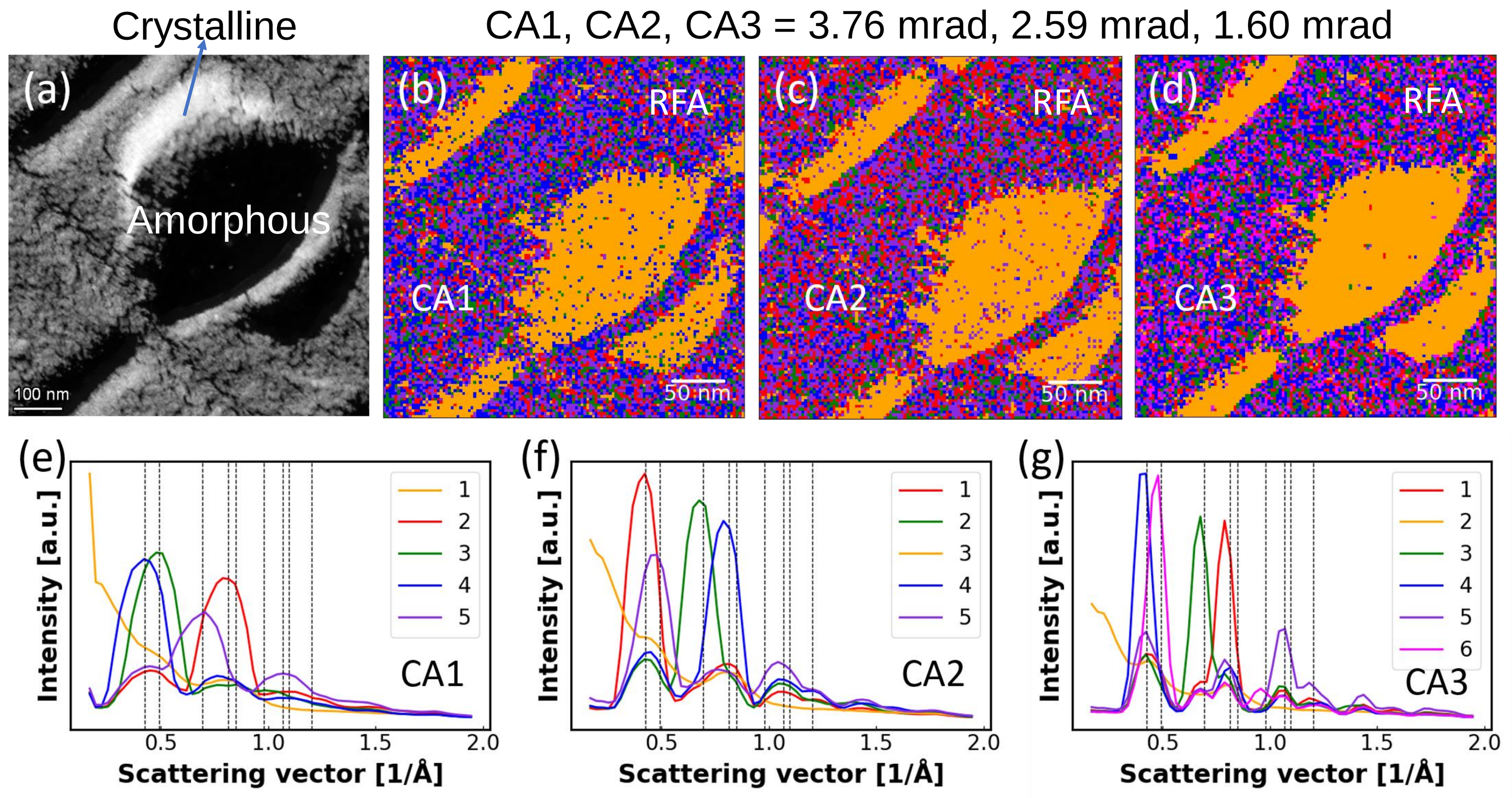
The method is tested under different experimental parameters to find the optimal experimental conditions.

The influence of the beam intensity



High intensity → good differentiation between crystal and amorphous phases

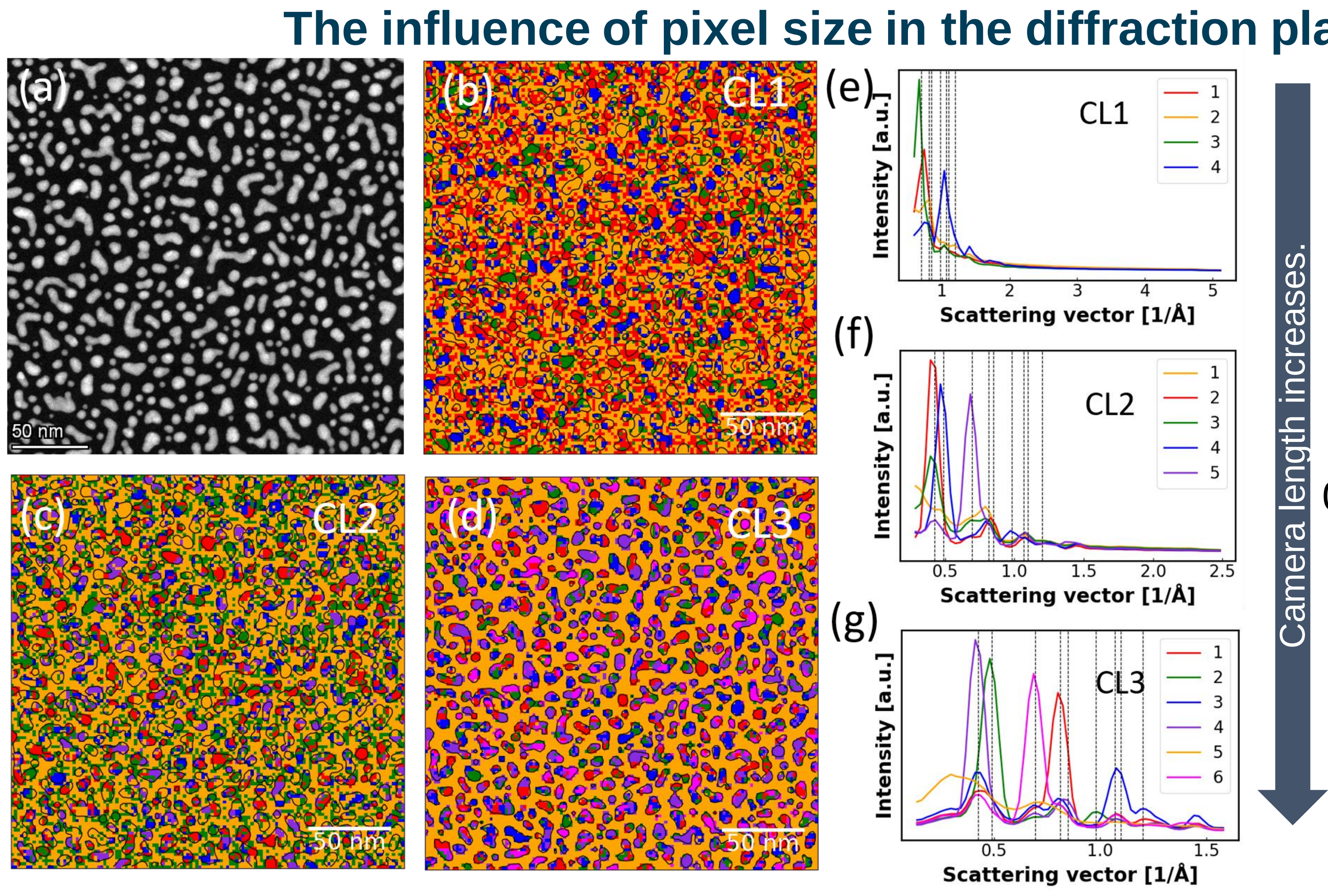
The influence of the convergence angle



Smaller convergence angle → sharper peaks

→ adjacent peaks (different orientation) can be distinguished

The influence of pixel size in the diffraction plane

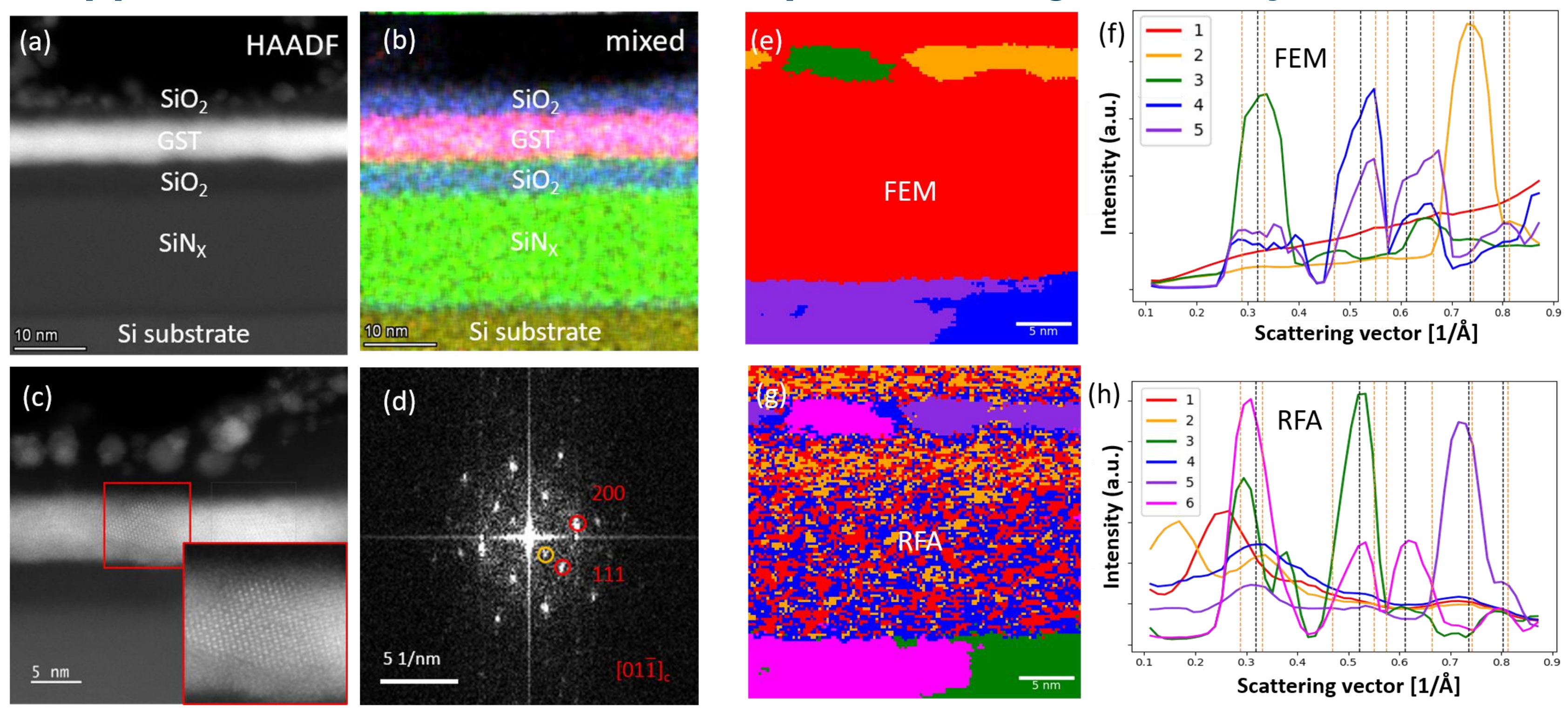


CL- Camera length

pixel size:
CL1 = 0.81(1/Å)/px
CL2 = 0.039 (1/Å)/px
CL3= 0.025 (1/Å)/px

Smaller pixel size in diffraction plane **→amorphous and crystal can be separated well → different orientation can be separated well**

Application of the method to the phase change memory materials



- Black dashed lines – the inverse d-spacings of Si
- Orange dashed lines – the inverse d-spacing of $Ge_2Sb_2Te_5$
- Crystalline clusters in the amorphous GST layer could be distinguished using both FEM and RFA based methods.
- Different amorphous phases (SiO_2 and SiN_x) can be distinguished by RFA

Conclusions

- A method to differentiate between amorphous and crystalline phases in the specimen is developed using 4D STEM. The concept of FEM and RFA is implemented to find the crystalline features in the diffraction patterns.
- The influence of the experimental parameters were studied. In general, larger beam intensity, smaller convergence angle, and relatively larger camera length lead to the reliable phase separation.
- Both FEM and RFA can distinguish successfully between amorphous and crystalline phases. RFA is found to be more robust to noise than FEM.
- The present method can be applied to study phase change mechanisms in different materials, ultimately during their resistive switching.

References

[1] C. Ophus, *Microsc. Microanal.*, **25**, 563, (2019),

[2] M. M. J. Treacy *et al.*, *Science*, **335**, 950, (2012).

[3]LiberTEM Authors., "LiberTEM Radial Fourier Series." https://libertem.github.io/LiberTEM/app/amorphous.html#radial-fourier-series.

[4]S. C. F. Lin *et al.*, *2014 11th International Conference on FSKD*, 814, (2014)

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