Measuring Strain at Sharp Interfaces Using 4D-STEM

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Abstract

Using 4-Dimensional Scanning Transmission Electron Microscopy, or 4D-STEM, we measured the strain at the silicon and germanium doped silicon interface, a material commonly used in transistors. The current best strain mapping technique is iterative ptychography, which relies on using a large convergence angle to create overlapping Bragg disks to reconstruct the sample phase. We are developing iterative Bragg ptychography that uses small convergence angle and has overlapping disks only when strain changes. Comparison of our method with old methods including correlation approach and differential phase contrast (DPC) on a simulated 4D-STEM sample has shown that iterative Bragg ptychography provided the highest resolution at the interface.

Keywords: 4D-STEM, ptychography, strain mapping

Introduction

Silicon and germanium doped silicon are widely used in transistors. Strain is the change in atomic distance with respect to the reference, or $\Delta x/x$. The sharp transition at the Si and Si-Ge interface creates unique strain pattern. To measure the strain, we used 4-Dimensional Scanning Transmission Electron Microscopy or 4D-STEM, in which an electron beam scans across a selected region in the sample, scatters through the sample, and forms a Bragg diffraction pattern at each scanned position. In a Bragg diffraction pattern, the distance between the Bragg disks is inversely correlated with the atomic distance, allowing strain mapping.

Methods

To compare the effectiveness of three straining mapping methods, we used python abTEM to simulate alternating sharp slabs of Si and Si-Ge (strained by 5% in the x direction) and collected 4D-STEM diffraction data. Then, the strain mapping methods were tested through python py4DSTEM. Afterwards, we collected 4D-STEM data on a real sample and ran the correlation approach and DPC.

Correlation Approach

We can compare the individual Bragg peak patterns with a reference to measure strain. Given a diffraction pattern, the location of the Bragg peaks can be identified through cross correlation with a reference Bragg peak called the kernel. We can calculate the average Bragg peak locations, set it as the reference, and calculate the difference with the individual Bragg peaks patterns. [1]

Differential Phase Contrast (DPC)

Differential Phase Contrast, or DPC, calculates strain by comparing the difference in exit wave phase, which is correlated with the atomic number. When the electron wave (ψ_0) interacts with the sample, it's scattered by the sample ($\psi_{exit}(\vec{r}) = \psi_0 \cdot e^{i\phi_0}$)**,** which is equivalent to a phase shift. The phase reconstructed from a Bragg peak depends on the local displacement. $\phi = G \cdot u$, where ϕ is the phase shift, G is the diffraction space position vector, and u is the lattice displacement. With some rearrangement, $\varepsilon_x = \frac{d\phi}{dx}/G_x$ and $\varepsilon_y = \frac{\mathrm{d}\phi}{\mathrm{d}y}/G_y$. For each of the Bragg peaks in a diffraction pattern, we located the center of mass, reconstructed the phase, and calculated the strain using the equations. [2][3]

Iterative Bragg Ptychography

The detector can only measure the intensity of the exit wave. At nonoverlapping disks, the intensity is phase independent. At overlapping disks, interference between the electron waves affects the intensity, causing observable phase dependence. Traditional iterative ptychography uses a large convergence angle for the beam and the Bragg peaks overlap in all scans. Our simulated sample uses a low convergence angle, so the Bragg peaks don't overlap. At the Si/Si-Ge interface, the diffraction peaks overlap due to the sharp transition, providing phase information. It then uses an iterative method to guess the sample wave, compare it with the data, and update the guess with a given step size. [2][3]

Results

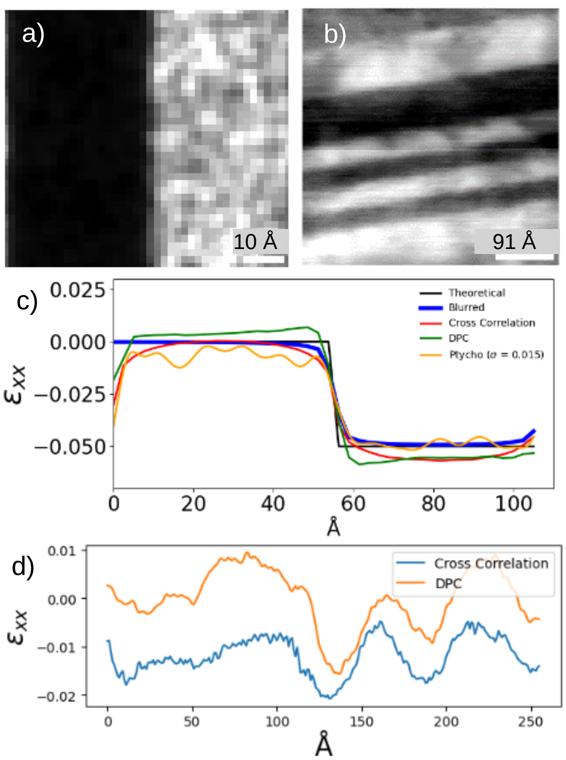

Fig 1. a) Si (black) / Si-Ge (white) Simulated Sample. b) Si (black) / Si-Ge (white) Experimental Sample. c) X Strain Map in Simulation. d) X Strain Map in Experiment.

In Fig 1 c), the blue blurred line is the realistic expected strain that accounts for the diffraction limit of the lens by convolving the strain map and the probe function. The highest resolution method has the latest drop in strain. From best to worst, the rank is iterative Bragg ptychography, DPC, and cross correlation. Despite the crucial role in ptychography, the overlapping disks at the sharp interface caused ineffective Bragg peak location identification in cross correlation, and hence low resolution.

Iterative Bragg ptychography had the best resolution. However, it has room for improvement. Known as Gibbs phenomenon, taking the Fourier transform of a function with a jump discontinuity (e.g., sharp strain change) results in fluctuations around the jump. We can find ways to smooth out the artifacts in the ptychography graph.

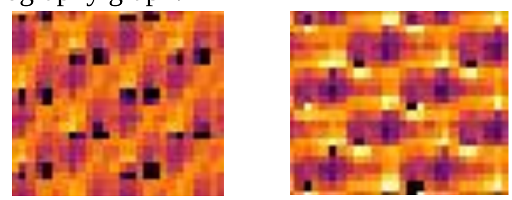

Fig 2. Ptychographic Reconstruction in Simulated Sample. Left: black dumbbell Si-Ge molecules. Right: obscure.

Additionally, shown in figure 2, the ptychographic phase reconstruction of the sample showed varying success with one place showing atomic details and the other hard to identify. This was resulted from the lack of disk overlap outside the sharp interface. However, at the sharp interface, this method worked well.

Shown in fig 1 d), experimentally cross correlation and DPC showed similar strain transitions through different layers, but the overall strain magnitude was different. More analysis is needed to measure the actual strain.

Future Work

We can explore ways to reduce the ringing artifacts in iterative Bragg ptychography, apply ptychography to experiments, and quantify the errors in our methods.

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Citation

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