TEM Lattice Calculator Documentation

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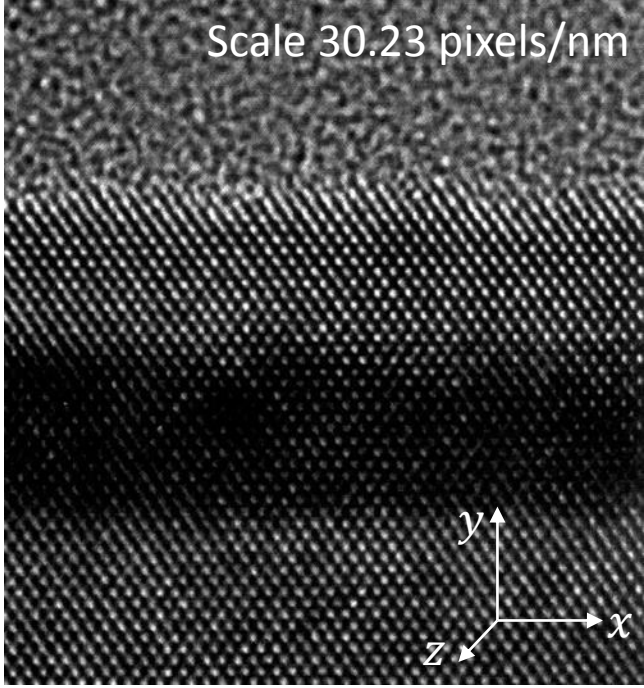
Example Input



- File *oxide_sSi_sGe_SiGe.png*: high resolution TEM image of an epitaxially grown heterostructure of Si, Ge, and SiGe
- The SiGe is relaxed meaning that it has zero strain in all 3 lattice directions
- The Si and Ge layers are strained to the lattice constant of SiGe in the x- and z- direction, but not in the y-direction since it is a free surface.

Strain and Lattice Constants

- Lattice constants, $a_{Si} = 0.5431$ nm, $a_{Ge} = 0.5658$ nm, $a_{Si_{0.7}Ge_{0.3}} = 0.5493$ nm
- Since the SiGe layer has a smaller lattice constant than Ge, the Ge is biaxially compressively strained in the x-z plane. This strain results in tensile strain in the y-direction due to Poisson's ratio.
- Since the SiGe layer has a larger lattice constant than Si, the Si is biaxially tensiley strained in the x-z plane. This strain results in compressive strain in the y-direction due to Poisson's ratio.

Lattice constants from http://www.ioffe.rssi.ru/SVA/NSM/Semicond/

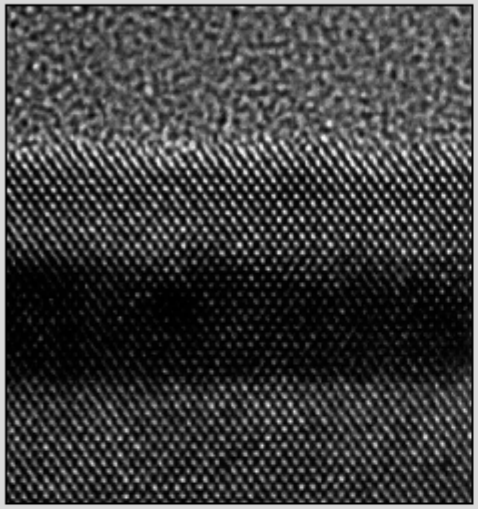
TEM Lattice Calculator | Terminate | Keep for later

1 Start → 2 Input TEM → 3 Scan Parameters → 4 Simulate

About this tool
Questions?

Rick click on the square next to "TEM Image" below to upload an image. The image will be used for computation of the local lattice constant. Most image formats should work.

TEM Image:



PNG image data, 500 x 535, 8-bit/color RGBA, non-interlaced
310.7 kB

The sample image is uploaded.

TEM Image Parameters

Scale of TEM (pixels/nm): **30.23**

Approximate lattice constant, a0 (nm): **0.5493**

Input the scale and approximate lattice constant.

Miller Crystal Directions

Define the Miller directions for the x- and y-directions of the image. The Miller direction is used to find the expected lattice planes through the equation, *d = a/sqrt(h^2+k^2+l^2)* where *d* is the spacing between (*hkl*) lattice planes, a is are the Miller indicies for a specific direction. The program finds *d* from the image and then calculates *a* using the afo

The program uses the approximate lattice constant as a starting point to find the actual lattice constant.

< Start | Scan Parameters >

Storage (manage) 9% of 1GB 780 x 600

TEM Lattice Calculator | Terminate | Keep for later

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About this tool
Questions?

TEM Image Parameters

Scale of TEM (pixels/nm): **30.23**

Approximate lattice constant, a0 (nm): **0.5493**

Miller Crystal Directions

Define the Miller directions for the x- and y-directions of the image. The Miller direction is used to find the expected lattice spacing between adjacent lattice planes through the equation, *d = a/sqrt(h^2+k^2+l^2)* where *d* is the spacing between (*hkl*) lattice planes, a is the lattice constant, and *h*, *k*, and *l* are the Miller indicies for a specific direction. The program finds *d* from the image and then calculates *a* using the aforementioned equation.

X-direction

h: **1**

k: **1**

l: **0**

Y-direction

h: **0**

k: **1**

l: **0**

< Start

Scan Parameters >

Storage (manage) 9% of 1GB 780 x 600

The x-direction in the image represents the $[1\ 1\ 0]$ Miller direction.

The y-direction in the image represents the $[0\ 1\ 0]$ Miller direction.

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Questions?

Below are parameters that specify the points at which to calculate the local lattice constant. The FWHM determines the size of the sample area of the original TEM image at the scan coordinate over which to compute the lattice constant. A larger value results in averaging over more lattice sites.

FWHM (nm): 2

Starting Coordinates

Starting x pixel coordinate for scan: 1

Starting y pixel coordinate for scan: 1

Ending Coordinates

Ending x pixel coordinate for scan: 201

Ending y pixel coordinate for scan: 501

Scan Step Parameters

Scan step size in x-direction (pixels): 50

Scan step size in y-direction (pixels): 5

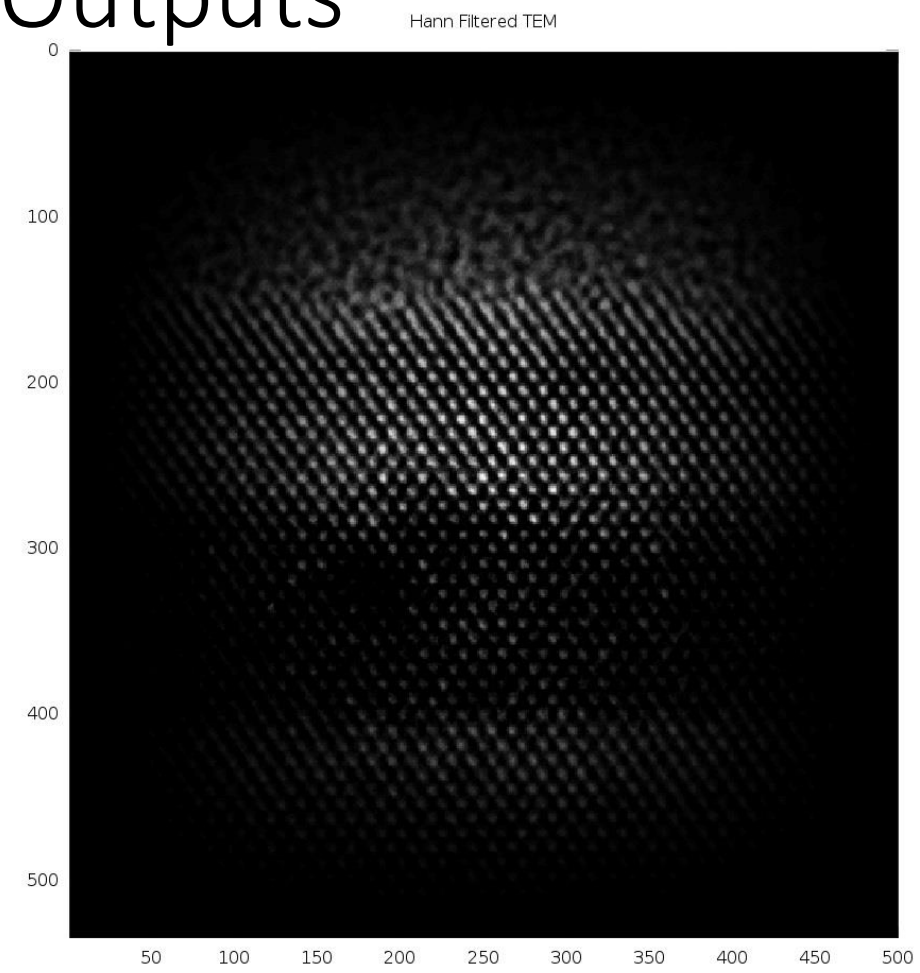
< Input TEM

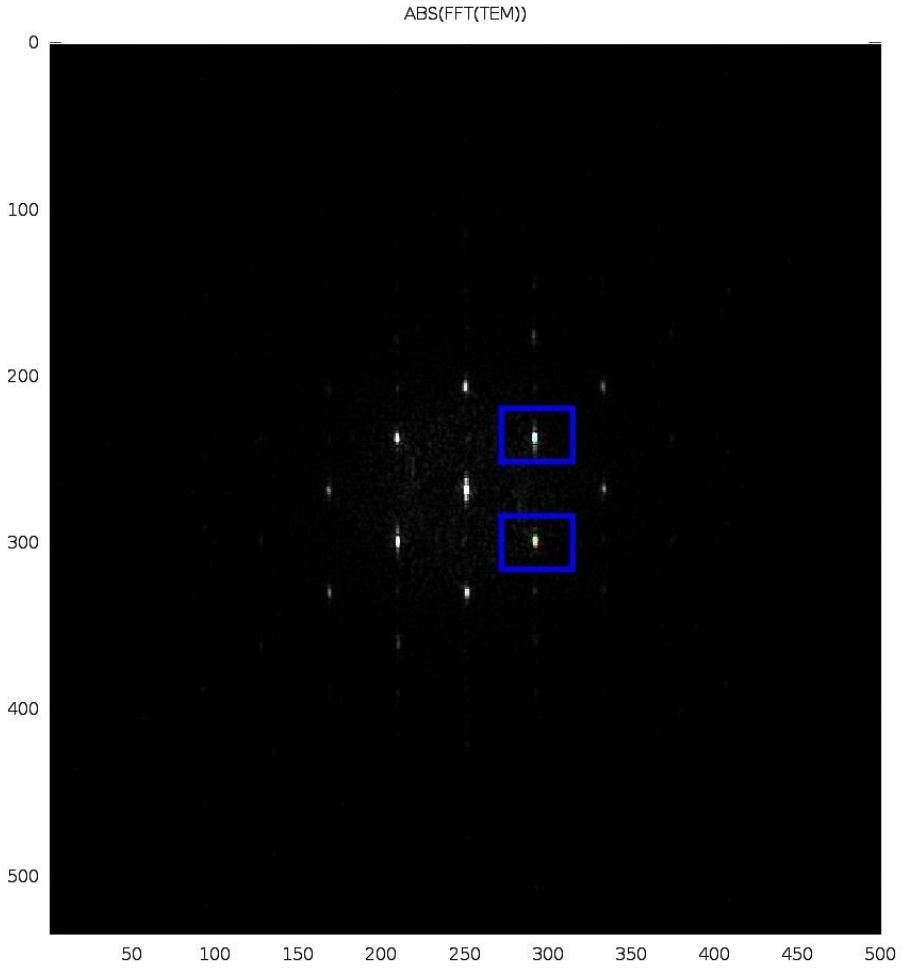
Simulate >

Storage (manage) 9% of 1GB

780 x 600

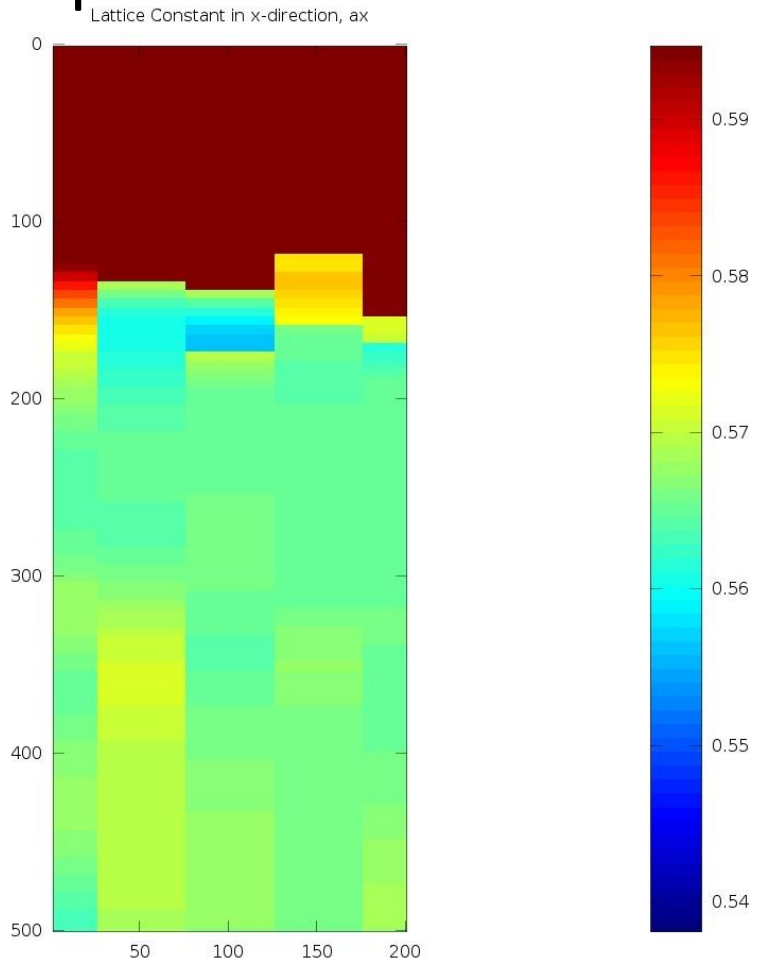
Outputs

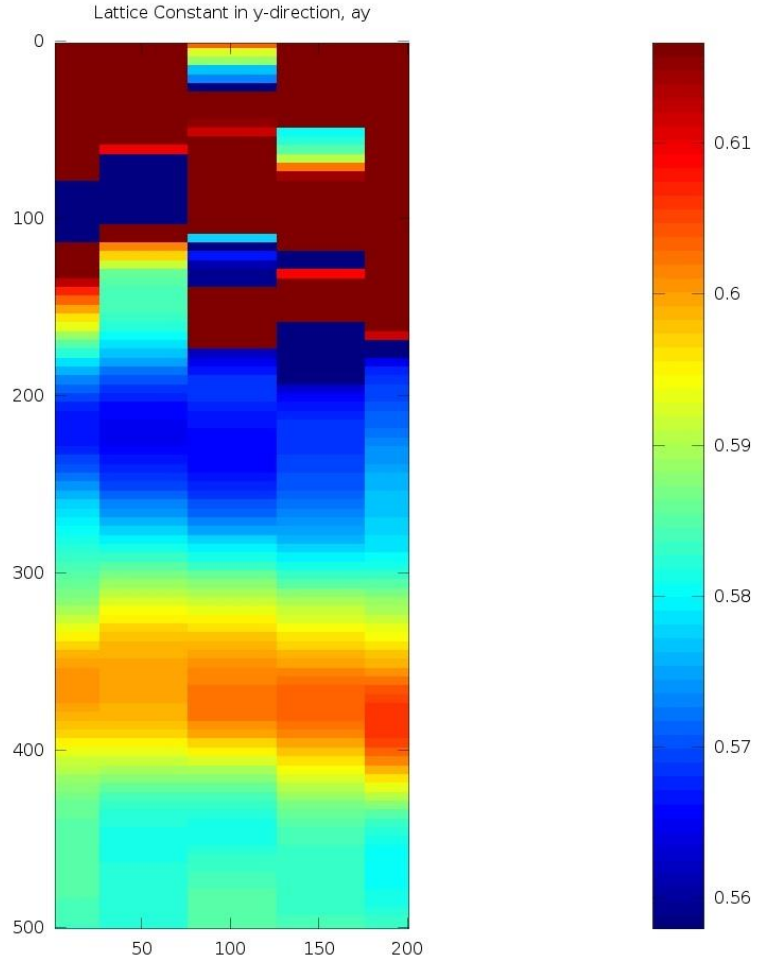




- *Hann Filtered TEM*: the original image with a Hann filter applied to it. The Hann filter is a sinusoidal function that decays to 0 at the edges of the image to reduce noise in the FFT.
- *ABS(FFT(TEM))*: the absolute value of the 2D Fourier transform of the Hann Filtered TEM. The blue boxes represent the areas over which the program searches for a maximum. The location of the maximum is related to the lattice constant. Zooming in reveals a red + and blue and green circles. The red + indicates the location of the *approximate* lattice constant entered in the input. The green and blue circles indicate the location of the actual maxima.

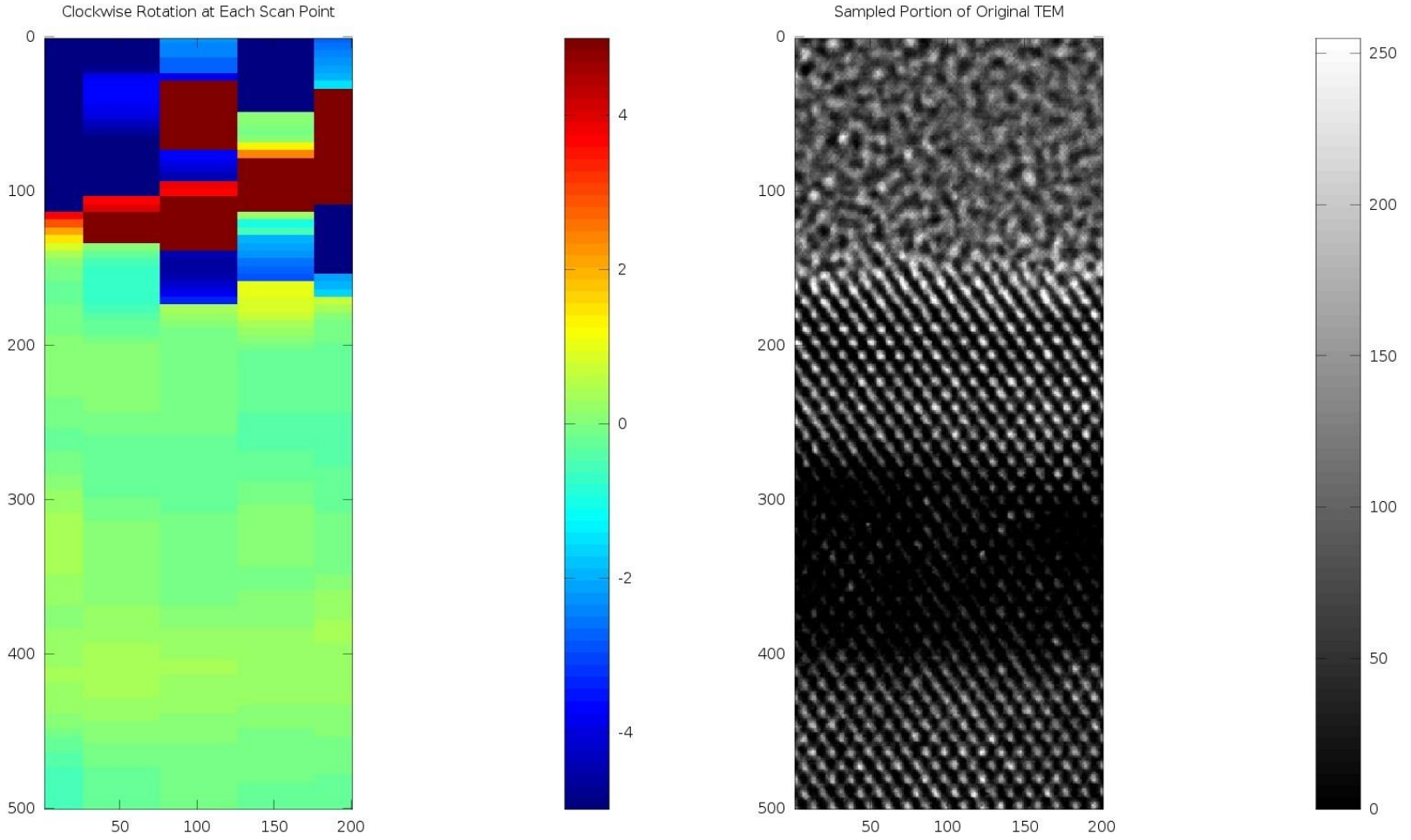
Outputs





- *Lattice Constant in x-direction, ax*: the lattice constant in the x-direction as a function of position in the image. The lattice constant in the x-direction is maintained in all the layers except the oxide, which is amorphous. Across the image, the average ax is ~0.565 nm which is quite large. This suggests that input value of image scale in pixels/nm should be adjusted to a slightly larger value such that $a_x \approx a_{Si_{0.7}Ge_{0.3}}$.
- *Lattice Constant in y-direction, ay*: the y-directed lattice constant is seen to vary substantially across the layers due to the strain.

Outputs



- *Clockwise Rotation at Each Scan Point*: the calculate rotation as a function of position. The rotation is calculated from the maxima of the FFT of the image at each point of the scan.
- *Sampled Portion of Original TEM*: the portion of the original TEM image over which the scan was performed. It can be useful in creating an overlay.