X-Ray Diffraction on Vertically Modulated Superlattices

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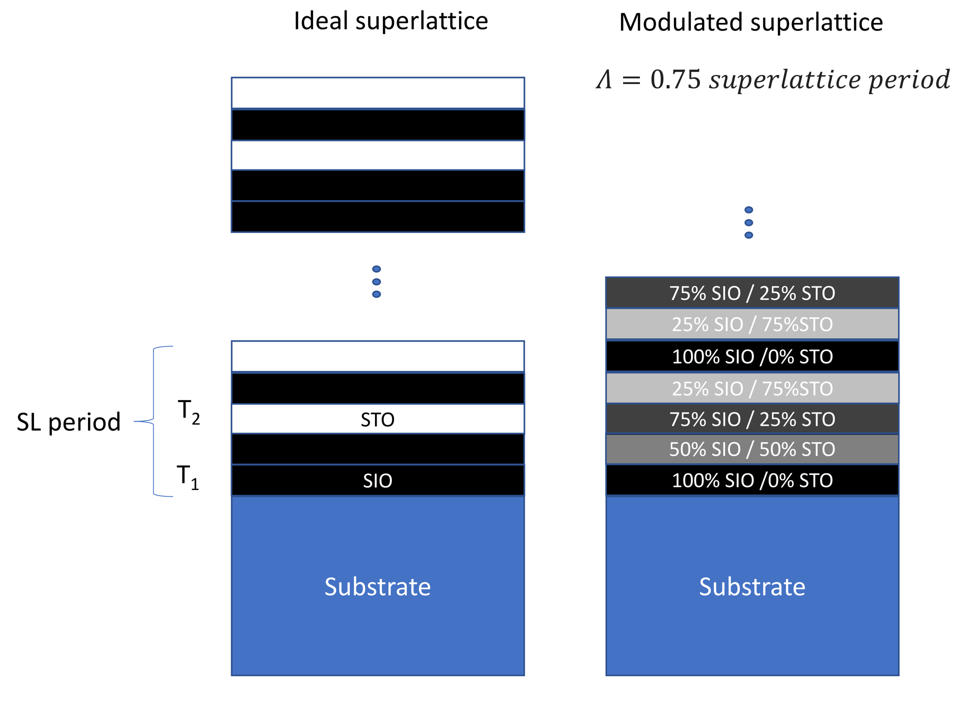
Modulated Superlattice



- Superlattice is a periodic structure of layers of two or more materials, these materials usually have similar microstructure.
- The superlattice is defined by the materials and atomic structure of each layer, the thickness of each layer, and the period of the superlattice.
- What is vertical modulation of the superlattice?
  - Period of vertical chemical composition is a noninteger multiple of the number of layers.
  - Defined by the wavelength of modulation (Λ).
- There are two ways this modulation can be formed:
  1) The chemical composition is homogenous in the lateral direction
  2) The chemical composition is changing in lateral direction, thus creating areas with different chemical compositions

Simulation of XRD on Modulated Superlattice

In the first case where the lateral composition is homogenous, the XRD can be calculated by the following model.

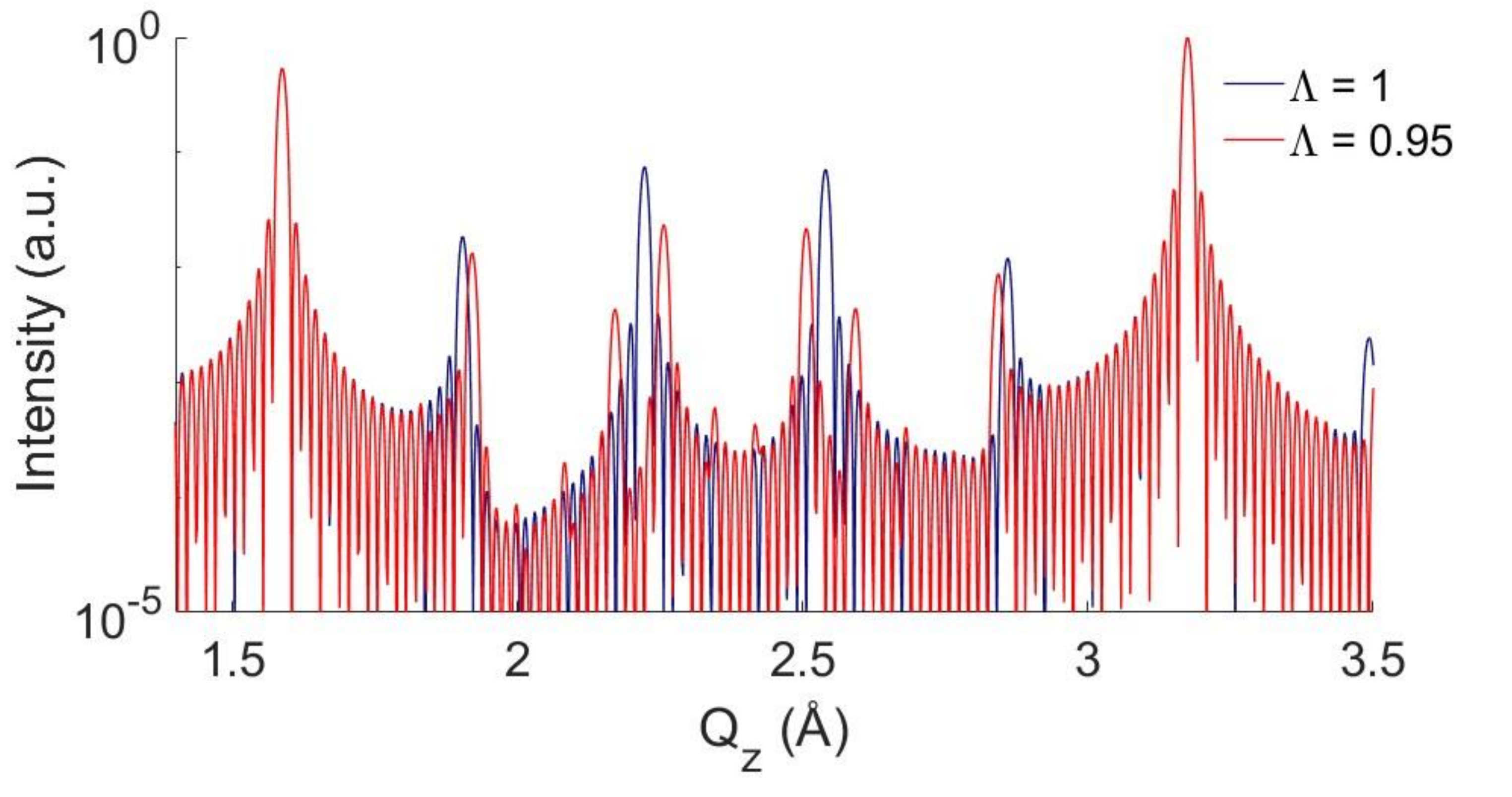
- Idea of the model:

1) calculate the occupancy in each layer from Λ

2) using the structure factors of individual materials, calculate the final structure factor of the superlattice as:

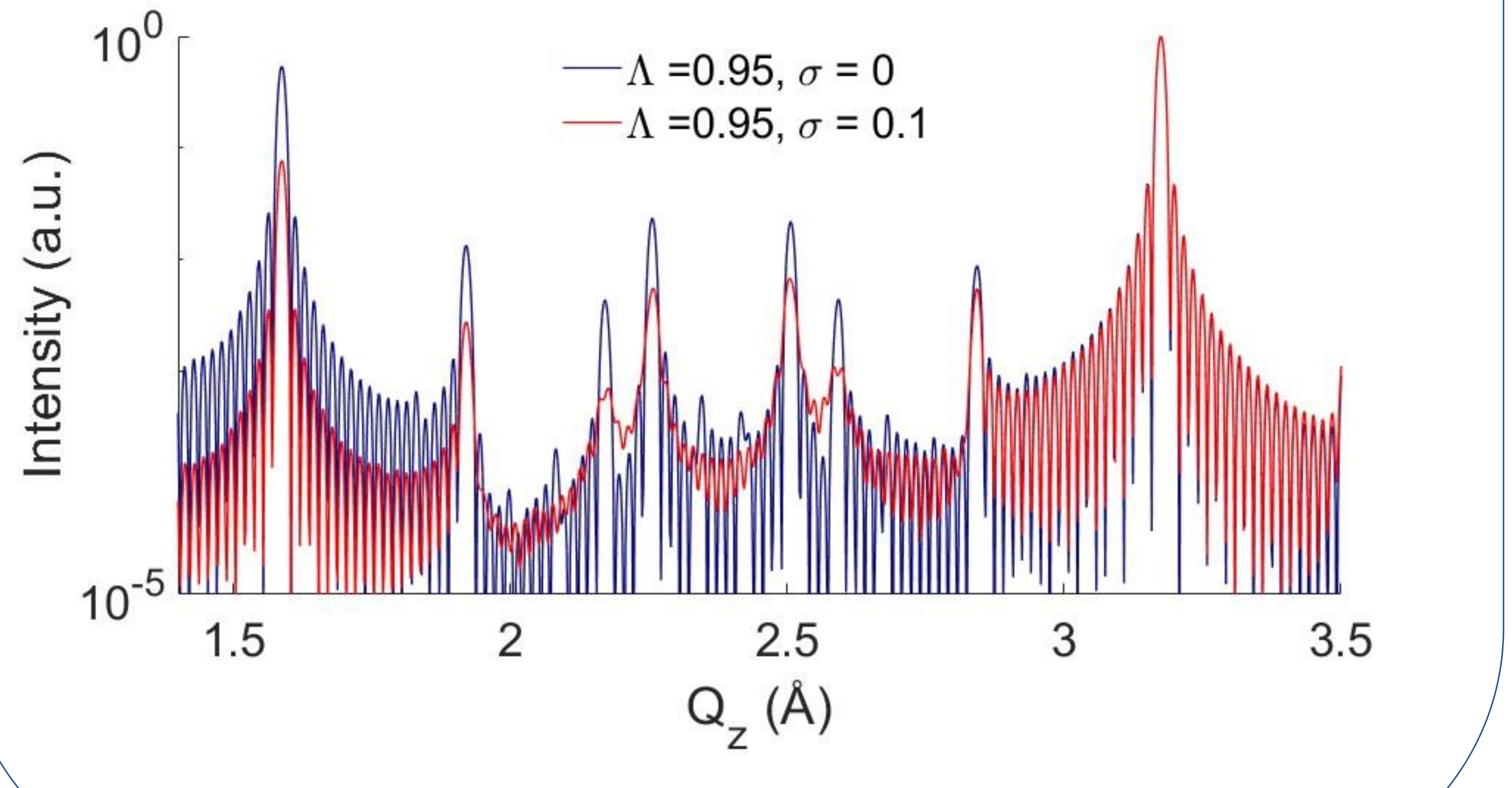
$F(Q_z) = \sum_j \left(x_{1j}F_1 + (1 - x_{1j})F_2\right) \cdot \exp(iQ_z z_j)$,

where x_{1j} is the fraction of sites occupied by material 1 in the j-th layer, z_j is the position of the j-th layer, and F_1 and F_2 are the structure factors of materials 1 and 2.



We observe a shift and splitting of superlattice peaks proportional to Λ.

This model can be modified for the second case where the chemical composition is changing in the lateral direction. Here we assume that the measured diffracted intensity is the sum of the intensities diffracted in areas with slightly different compositions. So, the measured intensity can be calculated as the sum of the intensities calculated by the previous model with a random component added to the occupancy of each layer. Lateral inhomogeneity can be characterized by the distribution of the random component. In the case of normal distribution, the important parameter is the standard deviation σ. Lateral inhomogeneity causes broadening of the superlattice peaks.



First Experiments

We measured superlattice with period $(SrIrO_3)_2/(SrTiO_3)_1/(SrIrO_3)_1/(SrTiO_3)_1$ deposited on $SrTiO_3$. The parameters obtained from the simulation are Λ=0.975 of the superlattice period and σ=0.1 of the superlattice period.