

# Detailed characterization of boron-rich nanostructures

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Methodology- A combination of techniques to understand the segregation behavior in the GB

- Thin and low damaged sample



- High resolution atomic HAADF imaging & model construction



- HAADF imaging simulation & HAADF image quantification

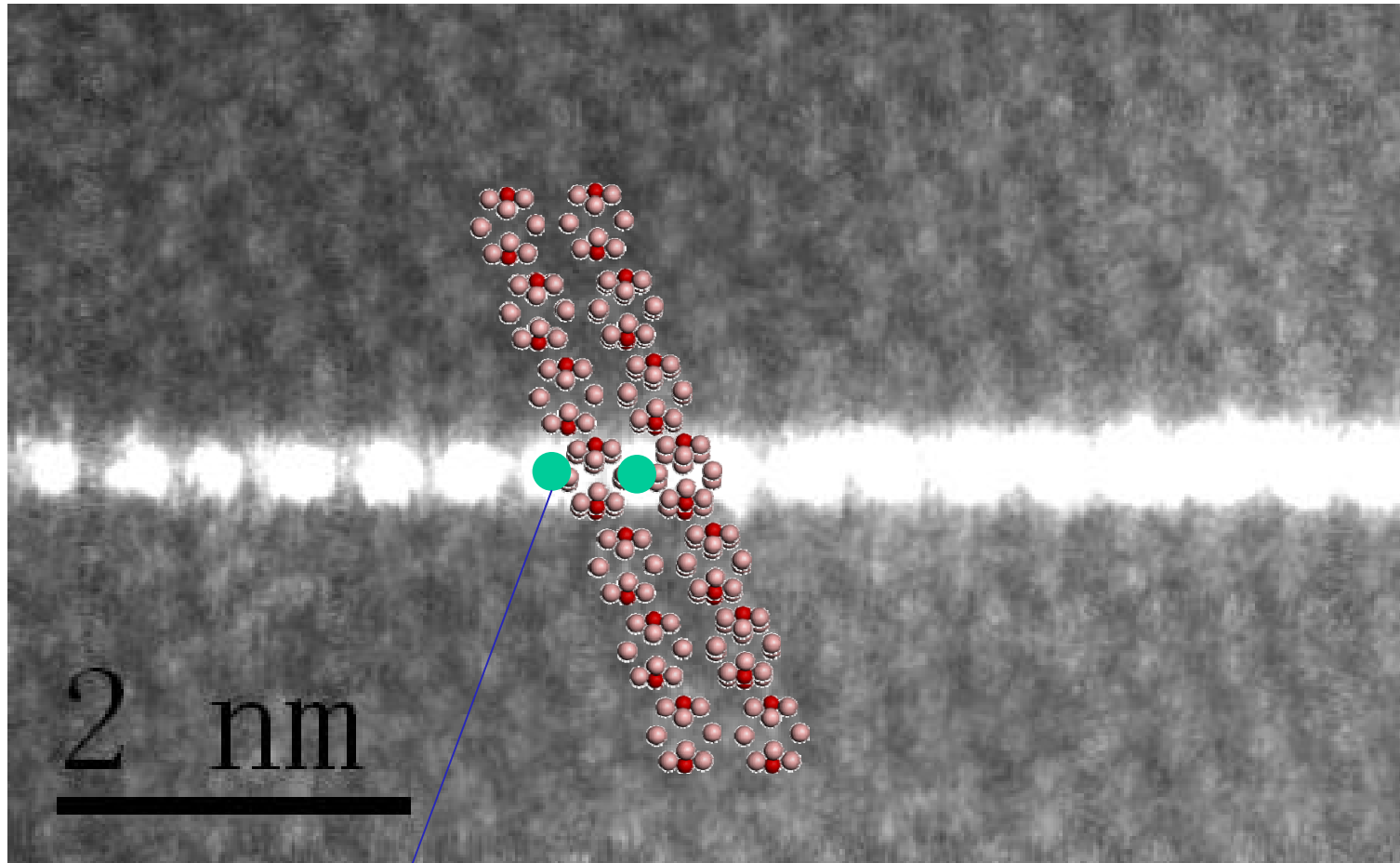


- DFT (First principle) simulation/molecular simulation/ Thermodynamic simulation



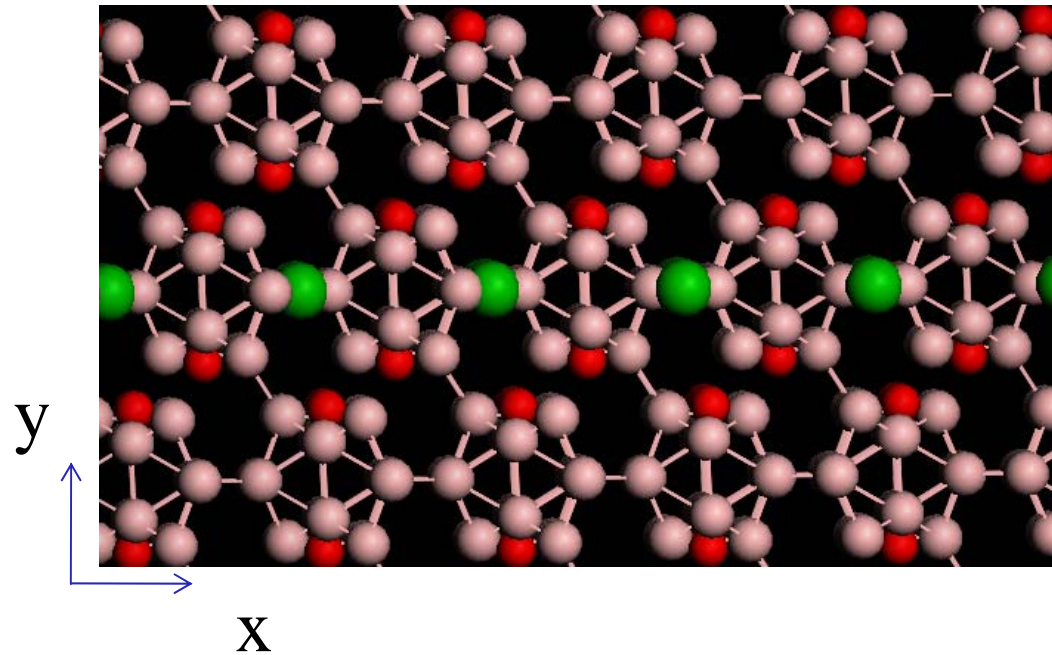
- Physical picture underlying

# 1.1 modeling of barium segregation



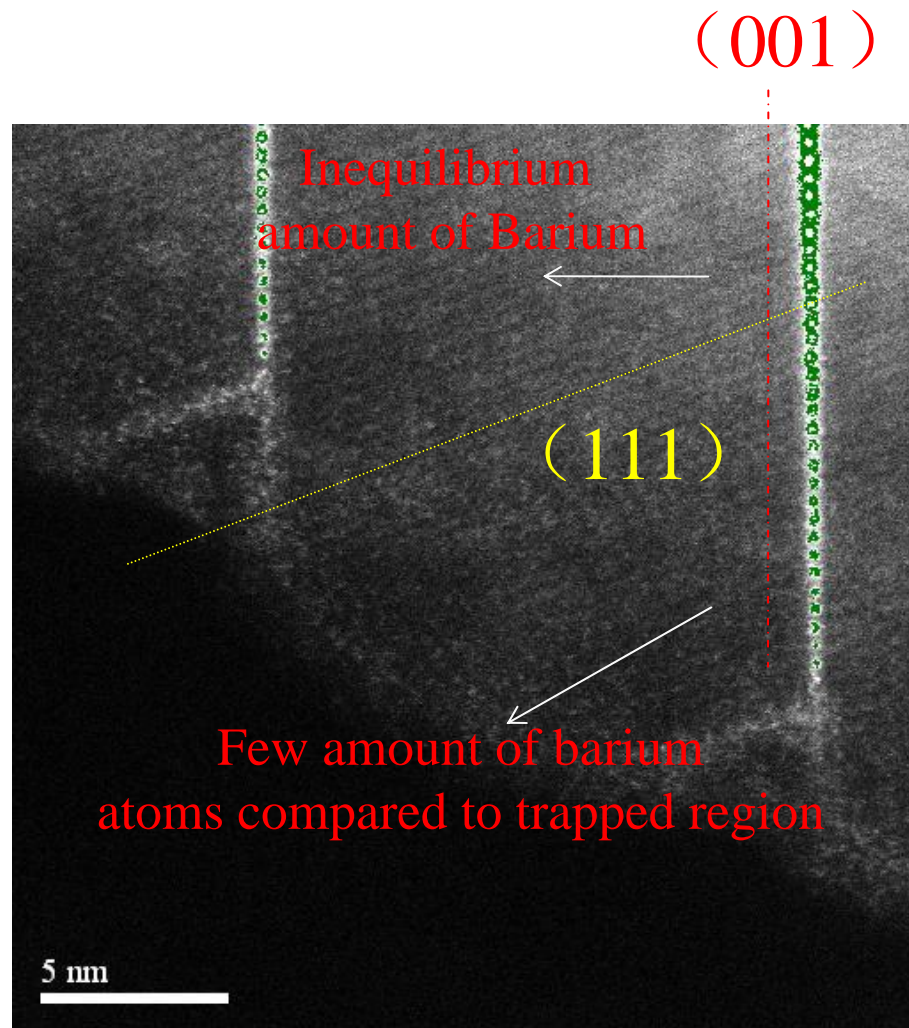
Extract Ba position

# 1.1 modeling of barium segregation



# 1.2 how many barium we have got? Quantification of HAADF image

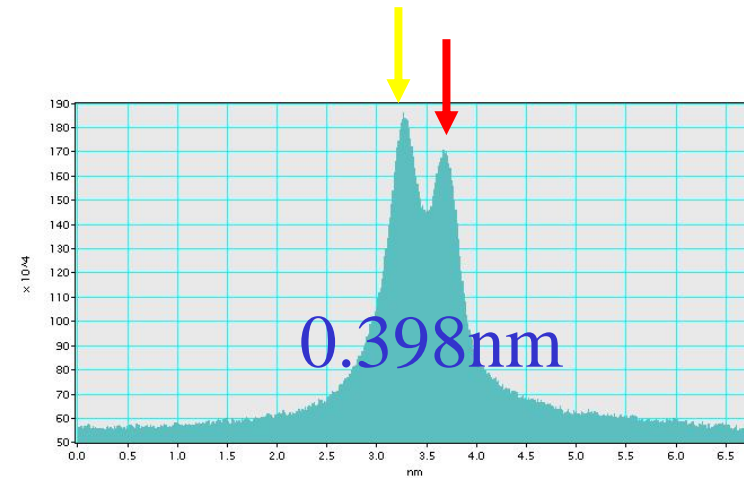
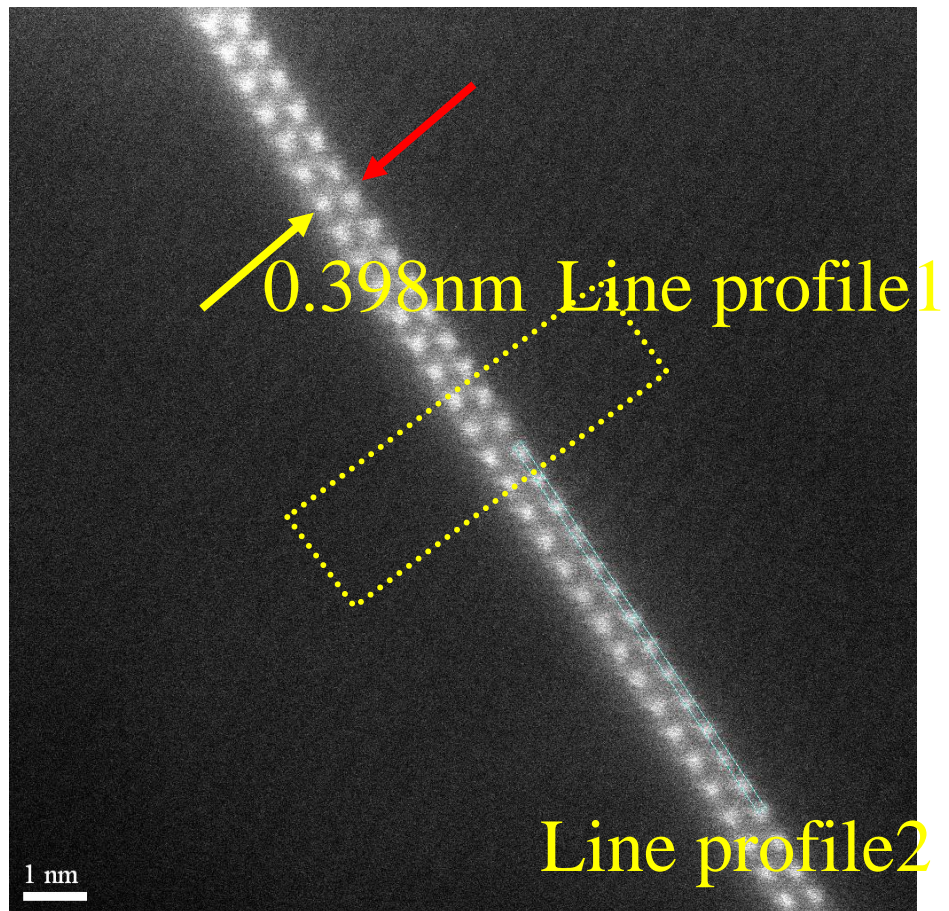
1200C nanowire  
Boron suboxide



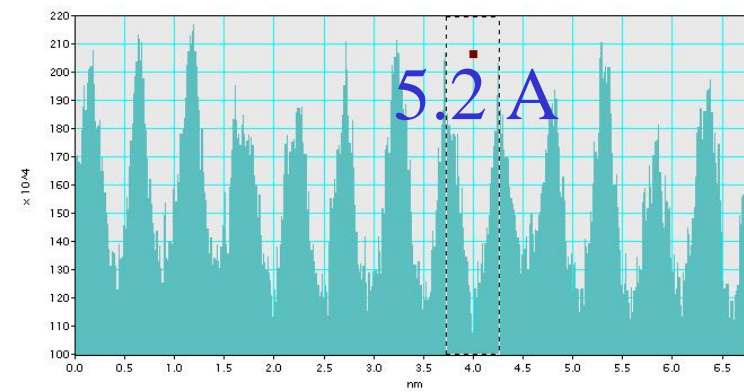
HAADF  
By Cs-corrected STEM in Lehigh University



## 1.3 Barium bilayer

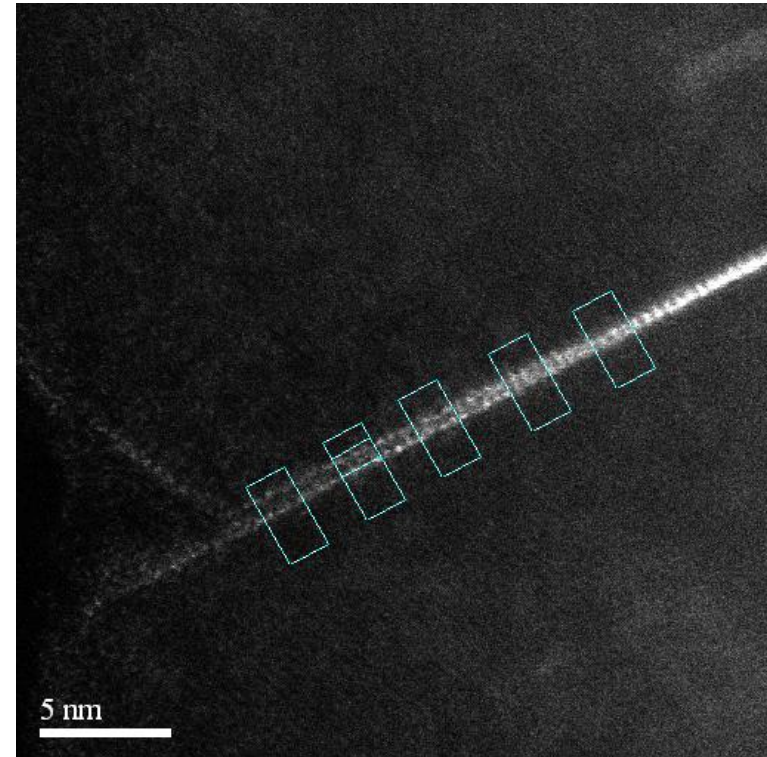
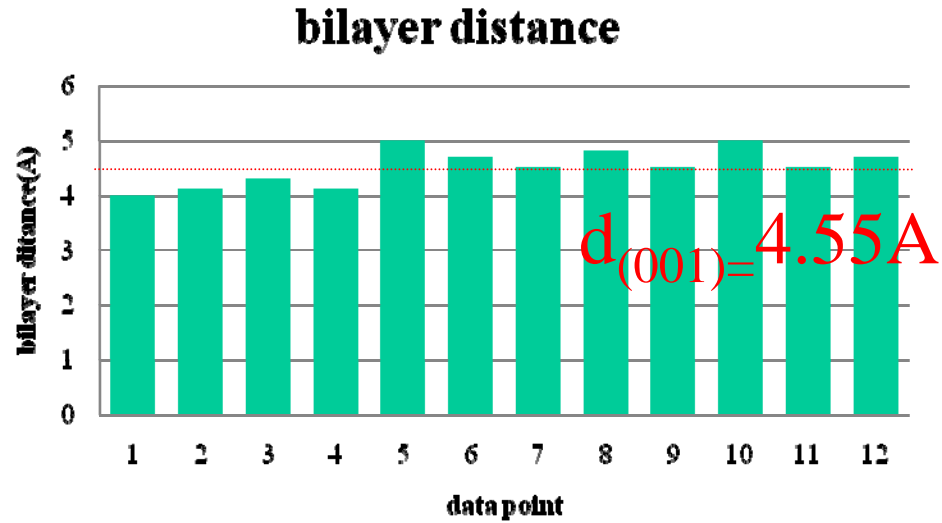


Line profile1

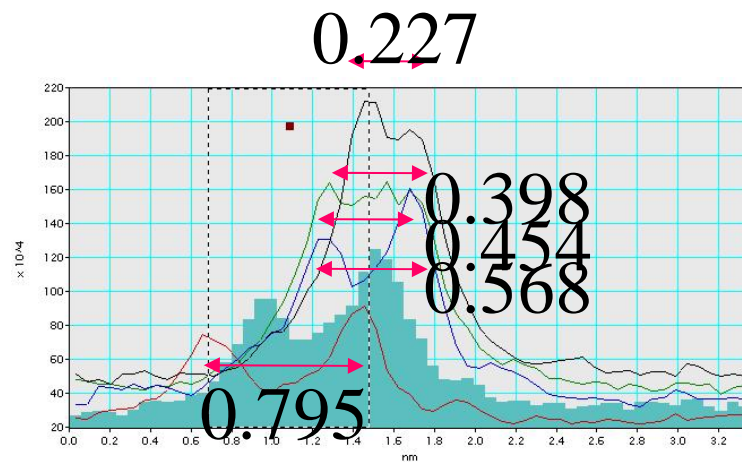


Line profile2

## 1.3 Barium bilayer



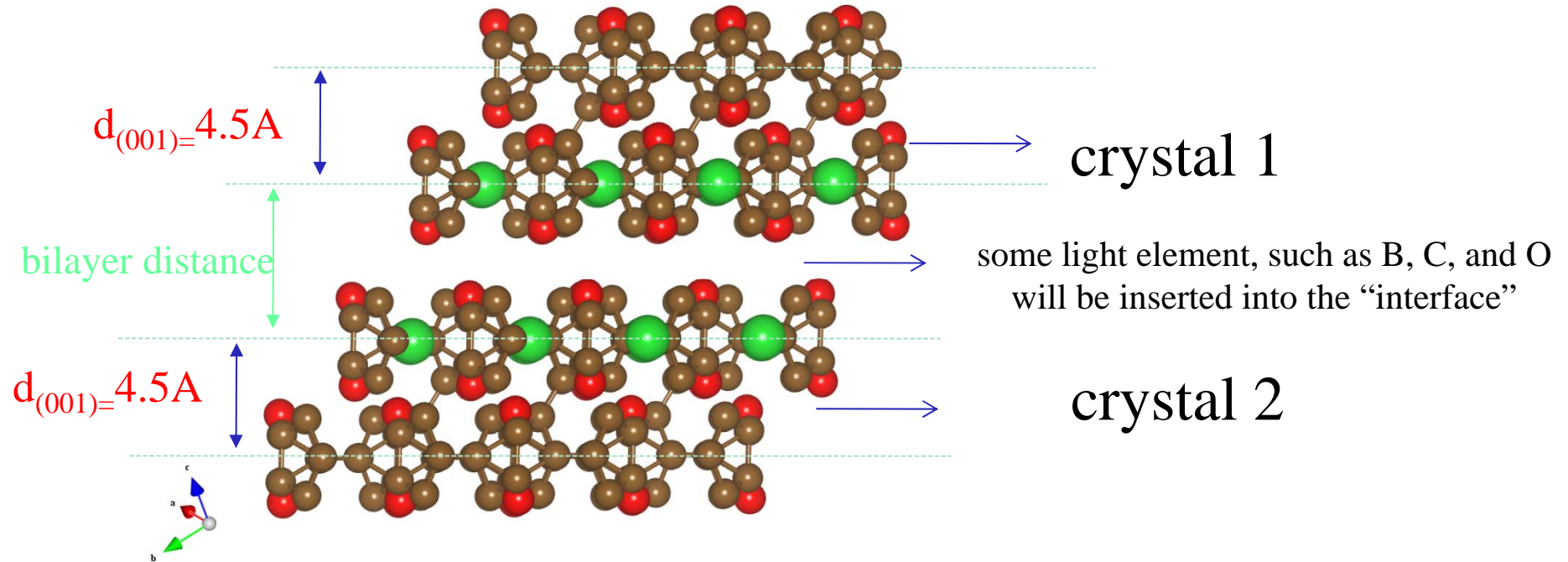
HAADF



line profile

Truly bilayer, one attached to upper crystal, and the other to the lower crystal

## 1.3 Barium bilayer-atomic configuration



A special but clear experiment proof  
of the existence of interface bilayer