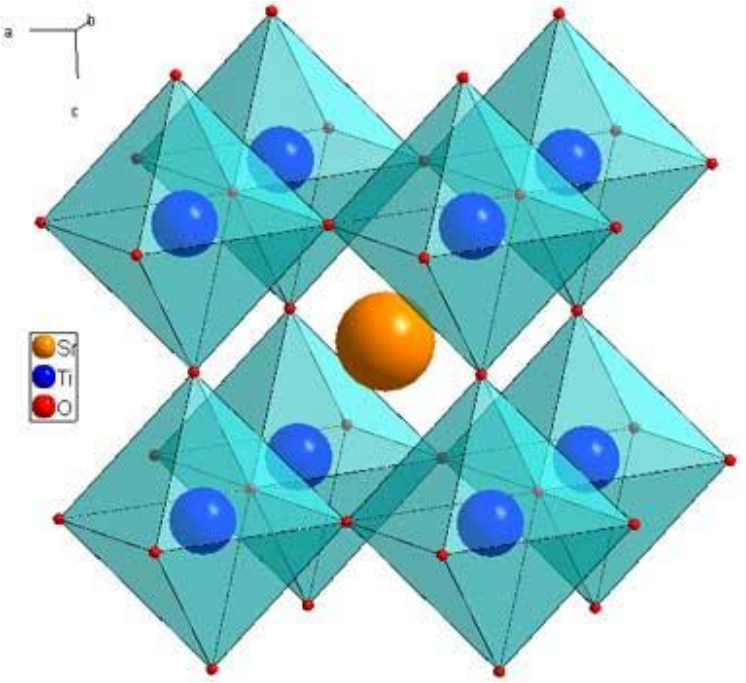
Direct imaging of $SrTiO_3$ surface reconstructions

M. Kruize

Journal club 6-11-2012

SrTiO3 crystal structure

- Cubic perovskite 0.3905 nm lattice parameter
- (001) SrO-TiO2 planes
  - Comparable thermodynamic stability
- Reconstruction surface
  - Ordered surface defect
  - Oxygen pressure and temperature related
- Many reported reconstructions of the 001 surface: (1x1), (2x1), c(4x4), c(4x2), c(6x2), (4x4) etc..



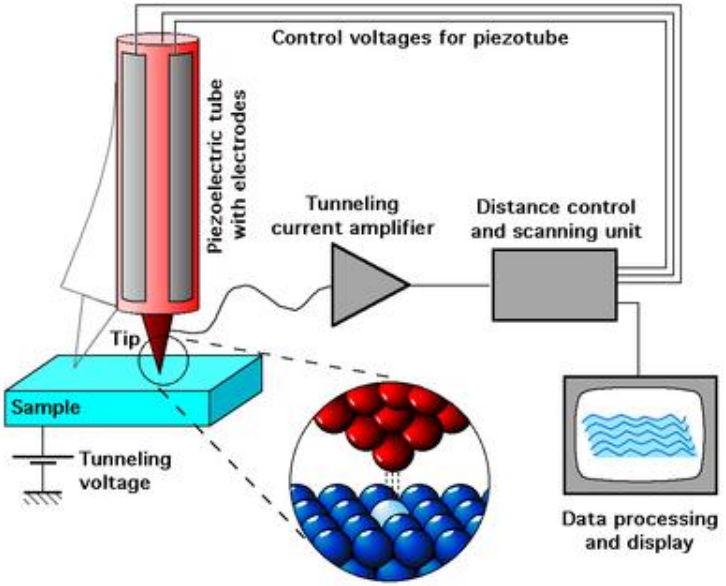
Scanning Tunneling Microscopy

- Conducting surface
  - Nb SrTiO3

- (1x1) 30 min @600 °C (10-8 Pa)

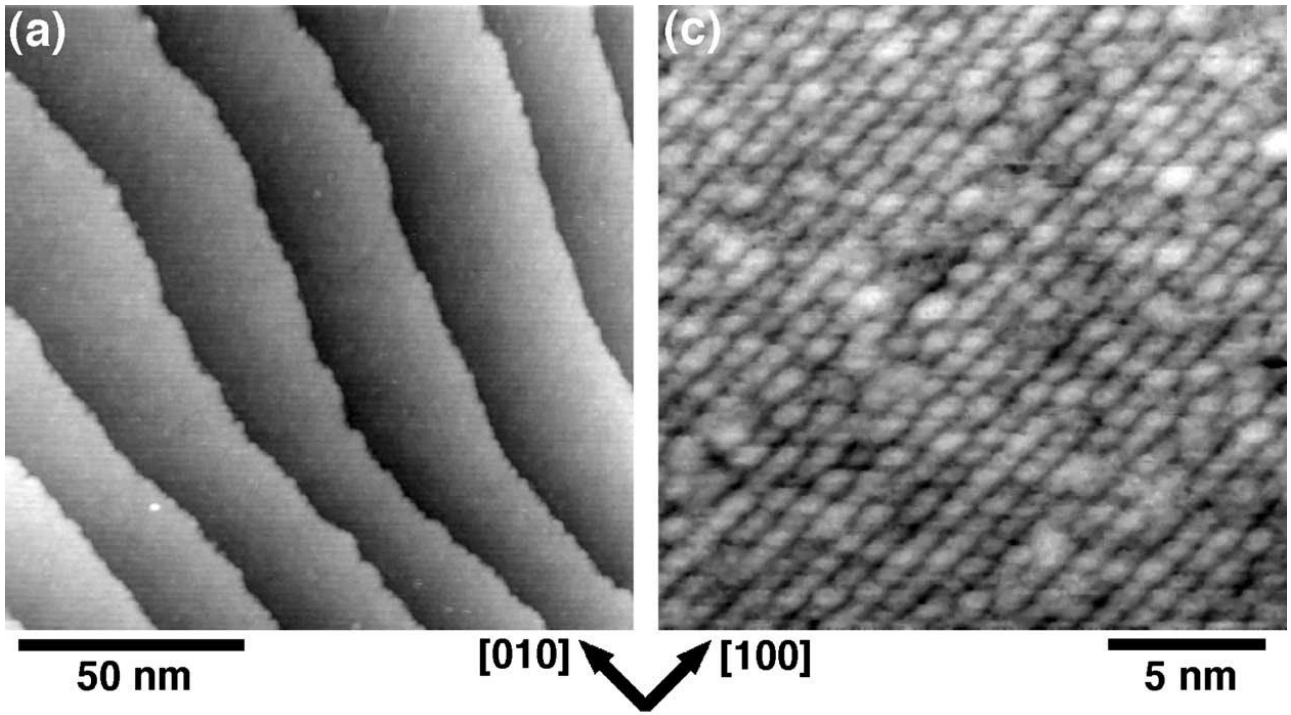
- (2x1) 30 min between 600-800 °C (10-8 Pa)

- c(4x4) 20 min @1100°C (10-8 Pa)



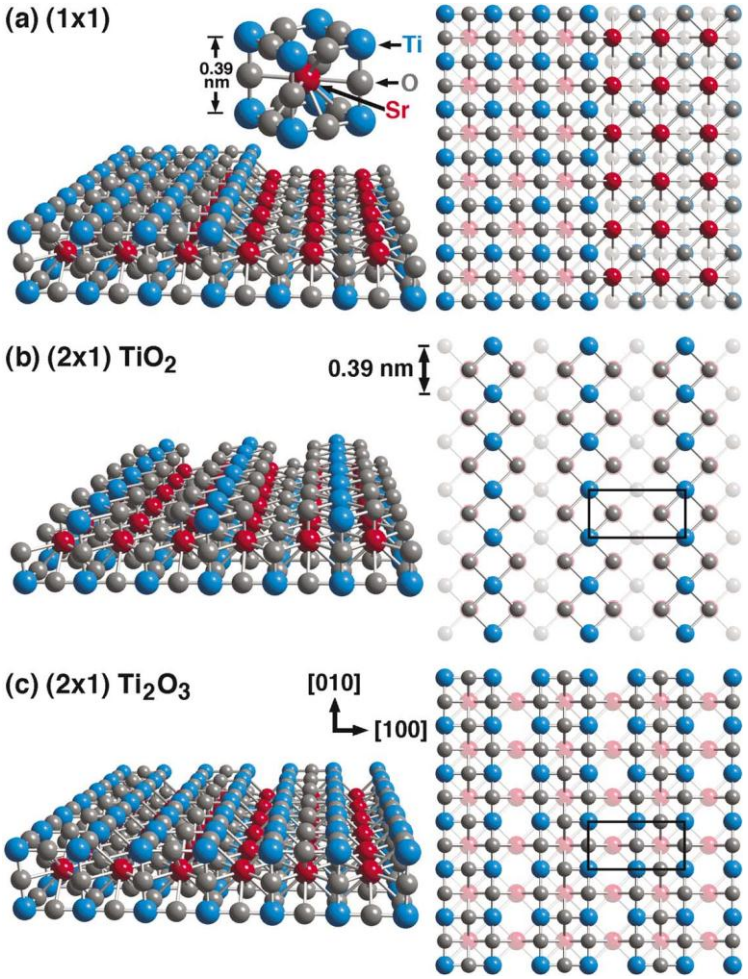
Castell, M.R. Scanning Tunneling Microscopy of reconstructions on the SrTiO3 (001) surface. *Surf. Sci.* **505,** 1-13 (2002)

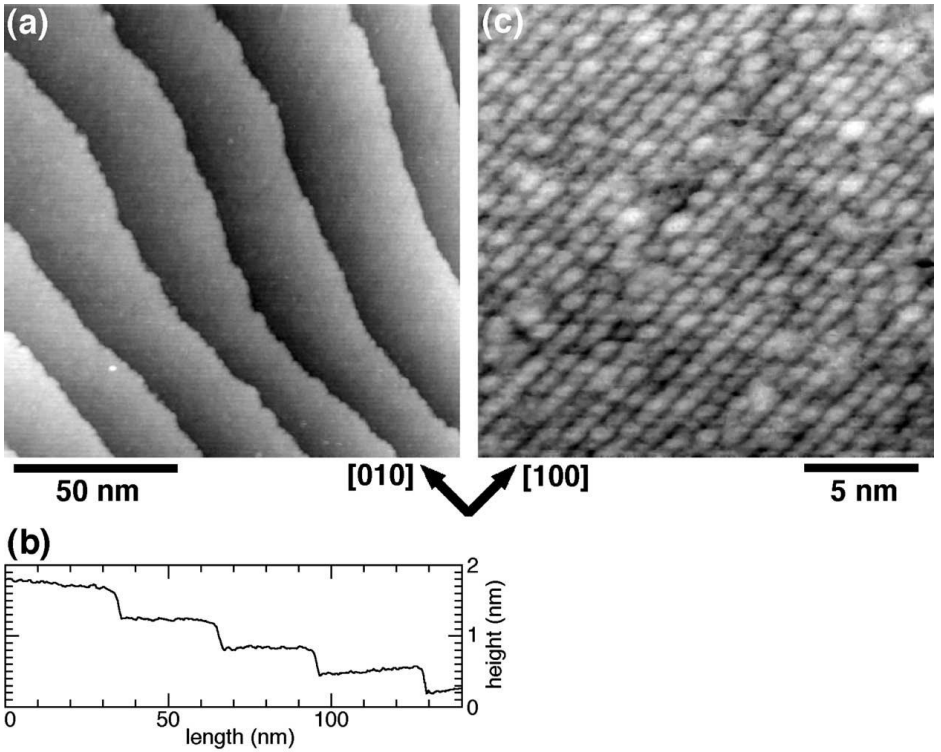
(2x1) surface reconstruction



Castell, M.R. Scanning Tunneling Microscopy of reconstructions on the SrTiO3 (001) surface. *Surf. Sci.* **505,** 1-13 (2002)

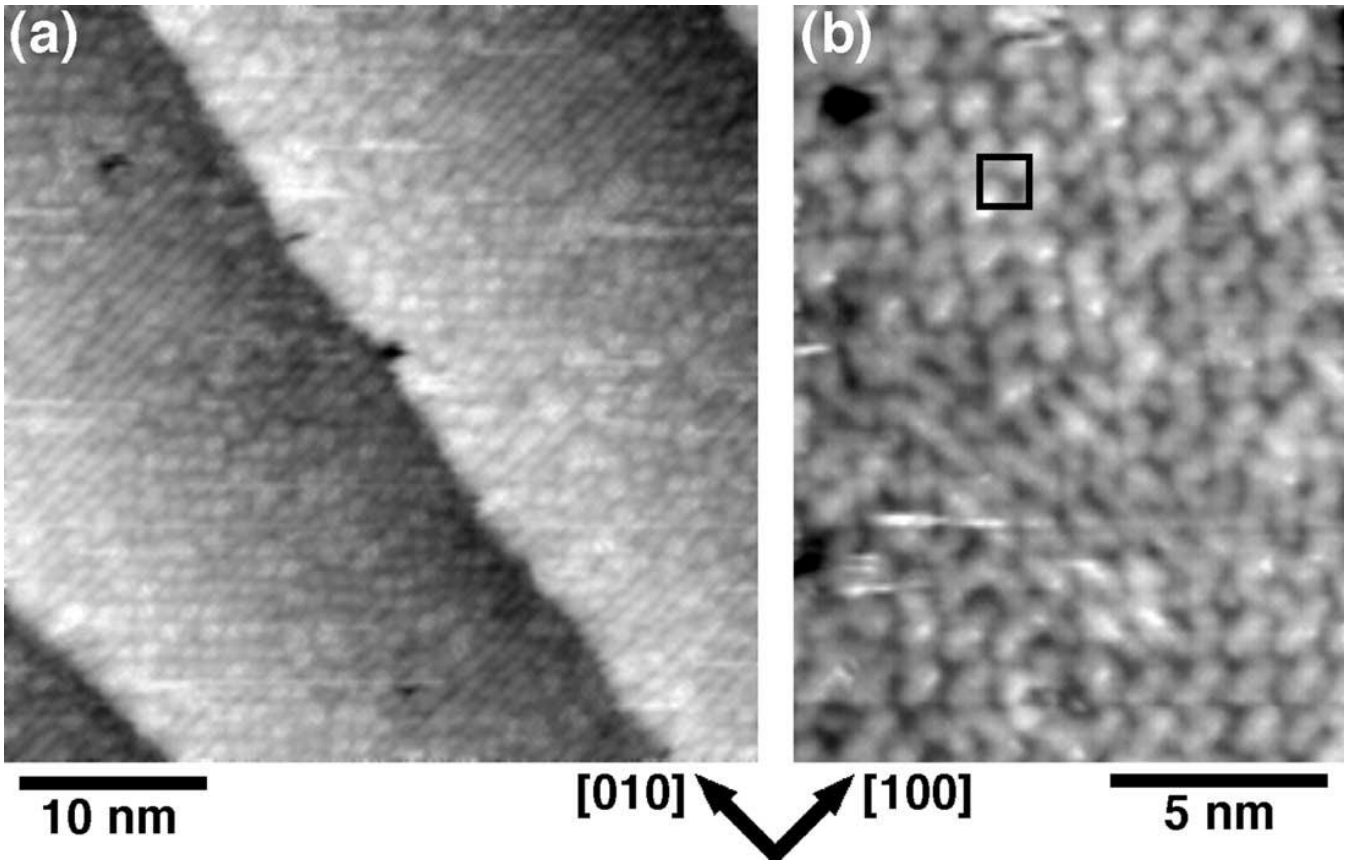
(2x1) surface reconstruction





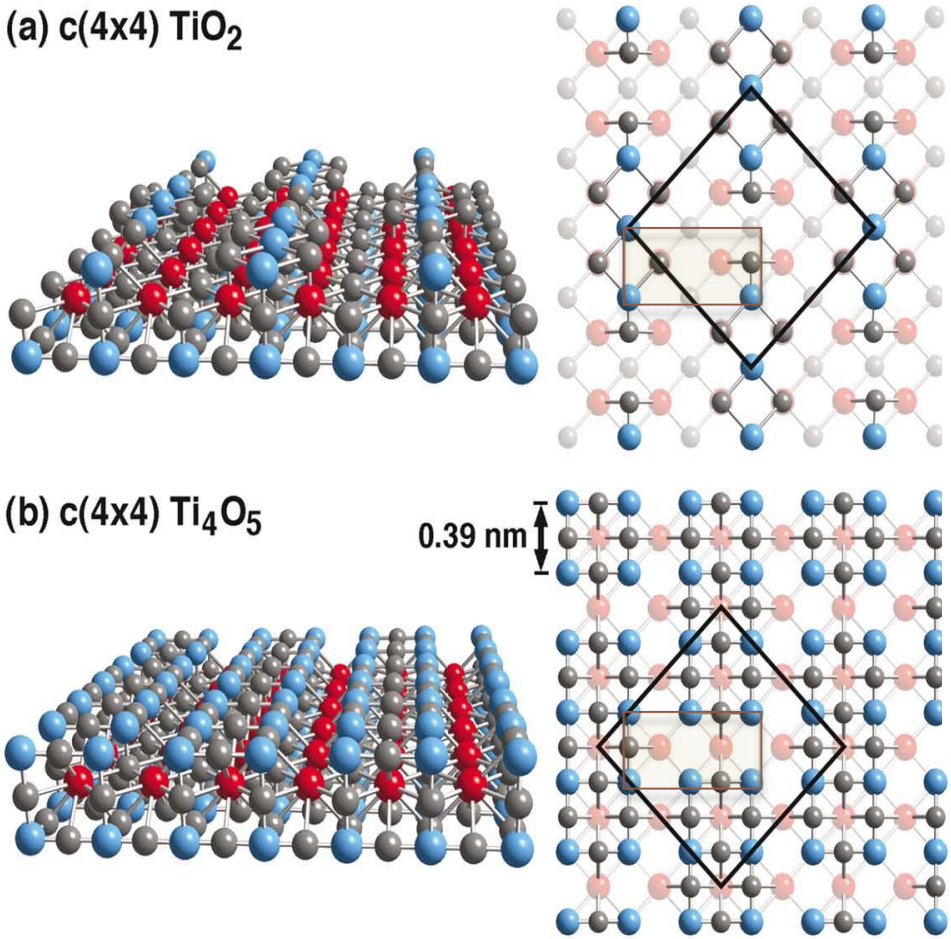
Castell, M.R. Scanning Tunneling Microscopy of reconstructions on the SrTiO3 (001) surface. *Surf. Sci.* **505,** 1-13 (2002)

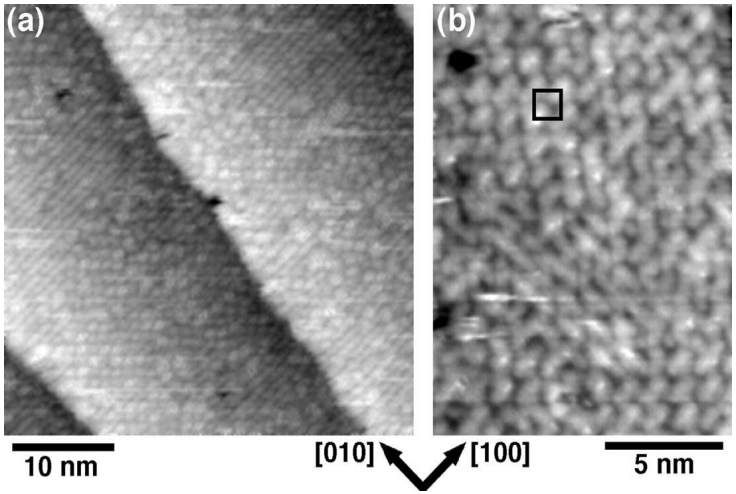
c(4x4) surface reconstruction



Castell, M.R. Scanning Tunneling Microscopy of reconstructions on the SrTiO3 (001) surface. *Surf. Sci.* **505,** 1-13 (2002)

c(4x4) surface reconstruction



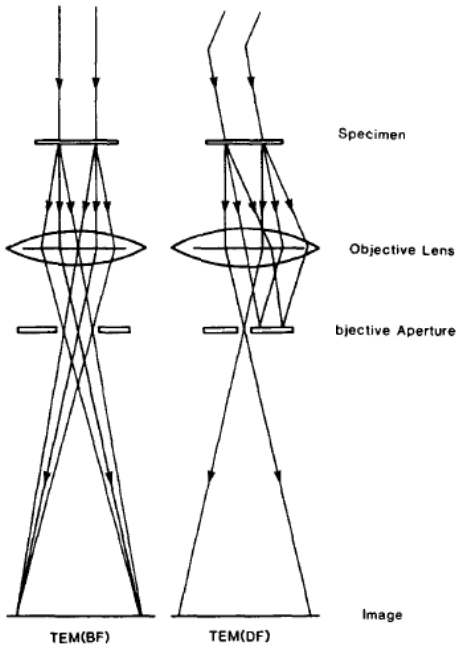


Castell, M.R. Scanning Tunneling Microscopy of reconstructions on the SrTiO3 (001) surface. *Surf. Sci.* **505,** 1-13 (2002)

Introduction TEM

- Bright field mode
  - Resolutions of angstroms
  - Imaging directly transmitted beam

- Dark field TEM
  - Incident beam tilted
  - Diffraction beam imaged
  - Crystal defect sensitivity



Cowley, J.M. Electron microscopy of surface structures. *Prog. Surf. Sci*, **21**, 209-250 (1986)

TEM: phase contrast of surfaces

- Primary contrast mechanism
  - Phase of incident electron wave is modified by distribution of electrostatic potential
  - If crystal is perfect, 100 nm thick one can reallign the sample to see surface
  - Surface steps, absorbed atoms or surface reconstructions visible if there are no bulk defects

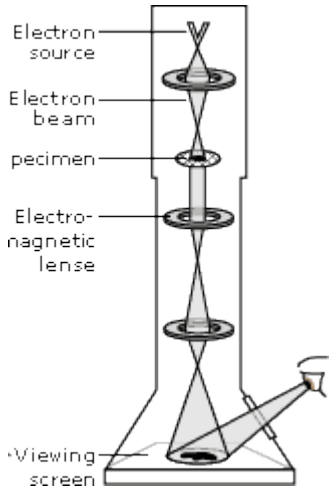
- Surface structural variations obscured by strong scattering in the bulk crystal

TEM: Dark field images with surface layer diffraction

- Need different periodicity of the surface compared to bulk
- Advantage is that it is relative insensitive to surface contaminations
- Images are very weak
  - Long exposure times: drift
  - Low resolution
  - Details of structure not seen

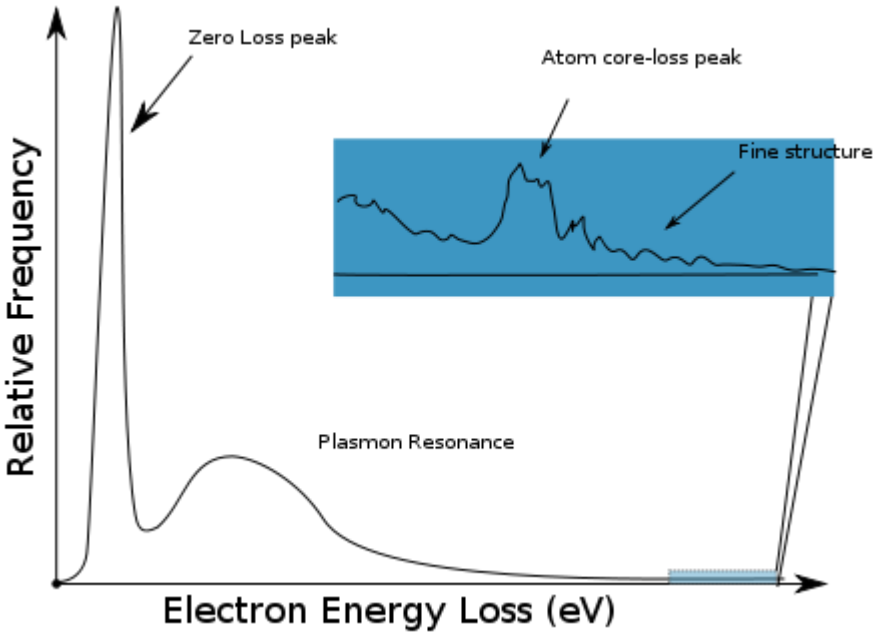
TEM: Nowadays

- Contrast formation
  - Bright field imaging mode
  - Electron diffraction contrast
  - Electron energy loss spectroscopy (EELS)
  - Phase contrast (HRTEM)
- Diffraction
- 3D imaging



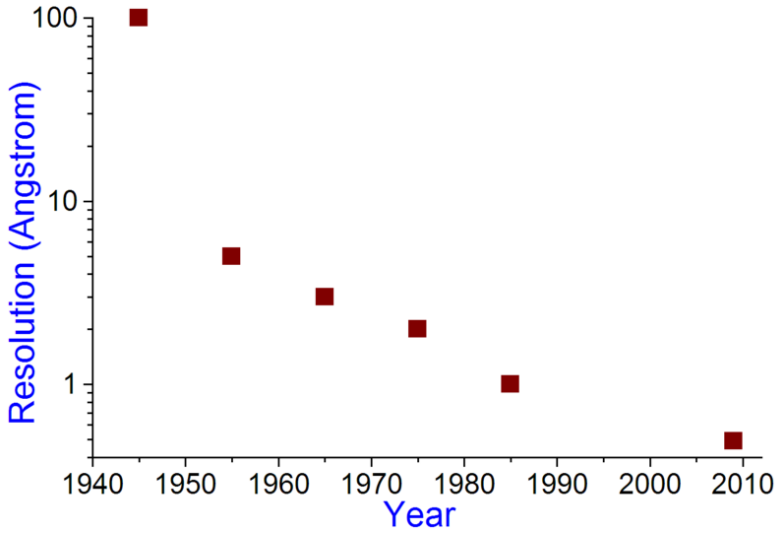
Electron Energy Loss Spectroscopy

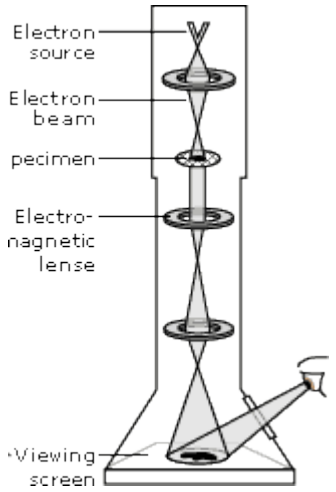
- Inelastic scattering
  - Phonon excitations
  - Inter and intra band transistions
  - Plasmon excitations
  - *Inner shell ionizations*
    - Type of atoms
    - Number of atoms
- Scattering angle
  - Dispersion relation
- Thickness measurements



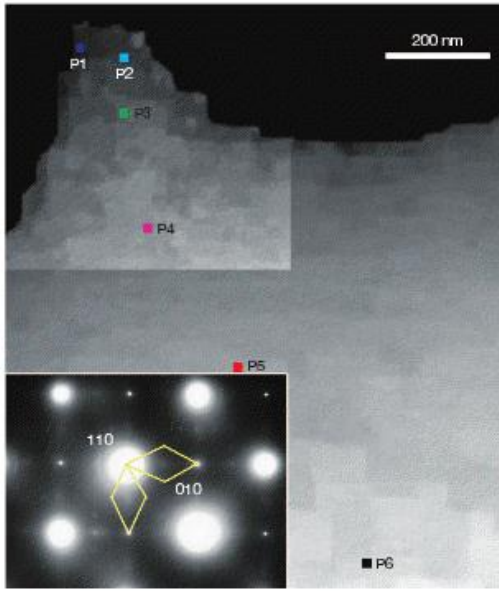
Transmission Electron Microscopy

- Limitations
  - Extensive sample preparation
  - Possible changing of the sample during prep
  - Small field of view
  - Sample damage due to beam
  - Resolution limits

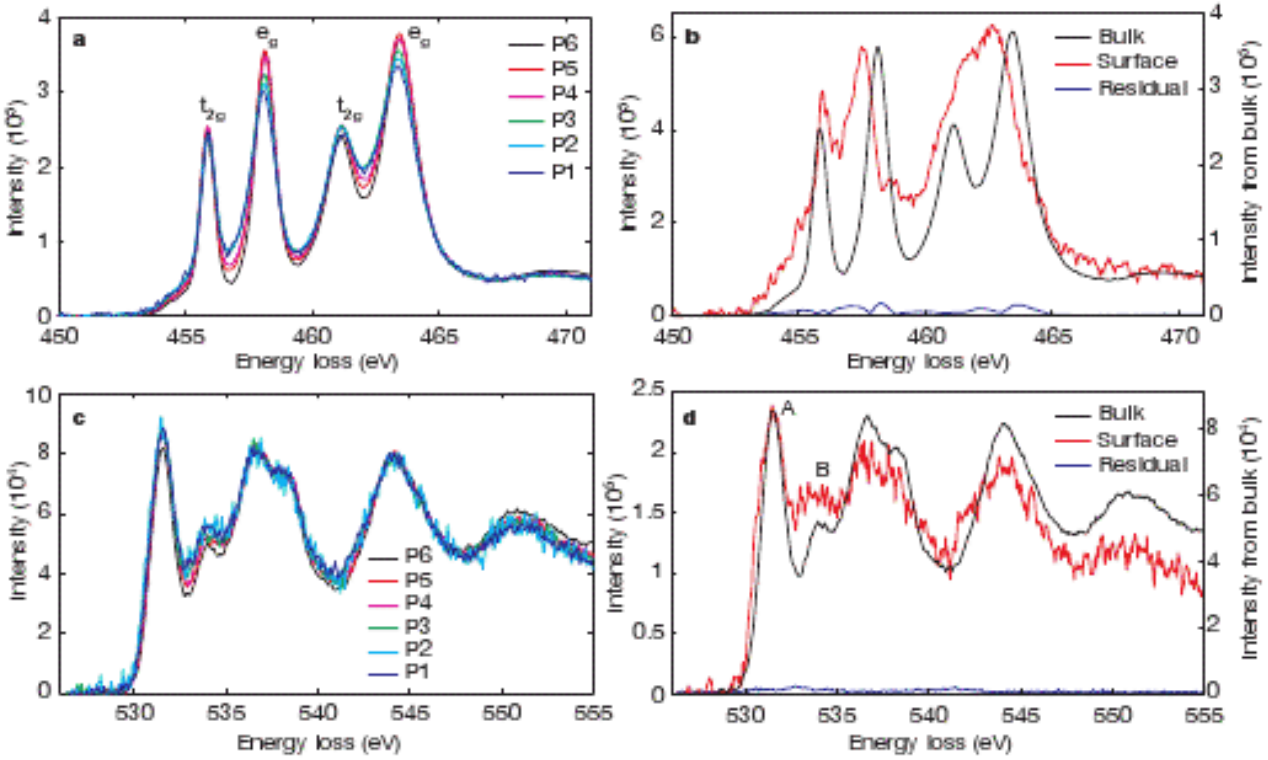




c(4x2): EELS

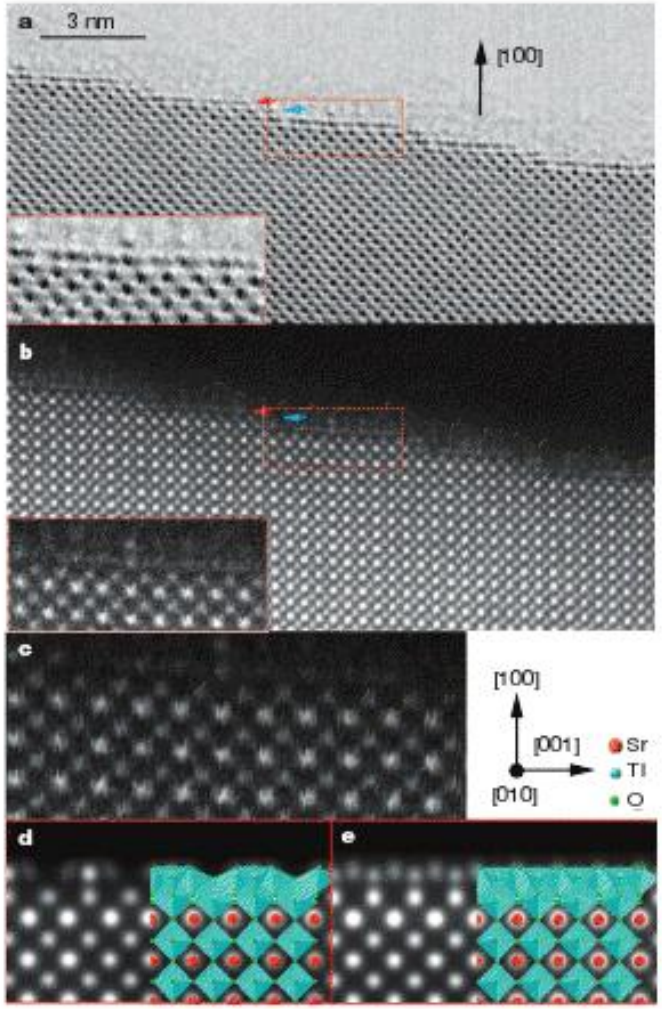


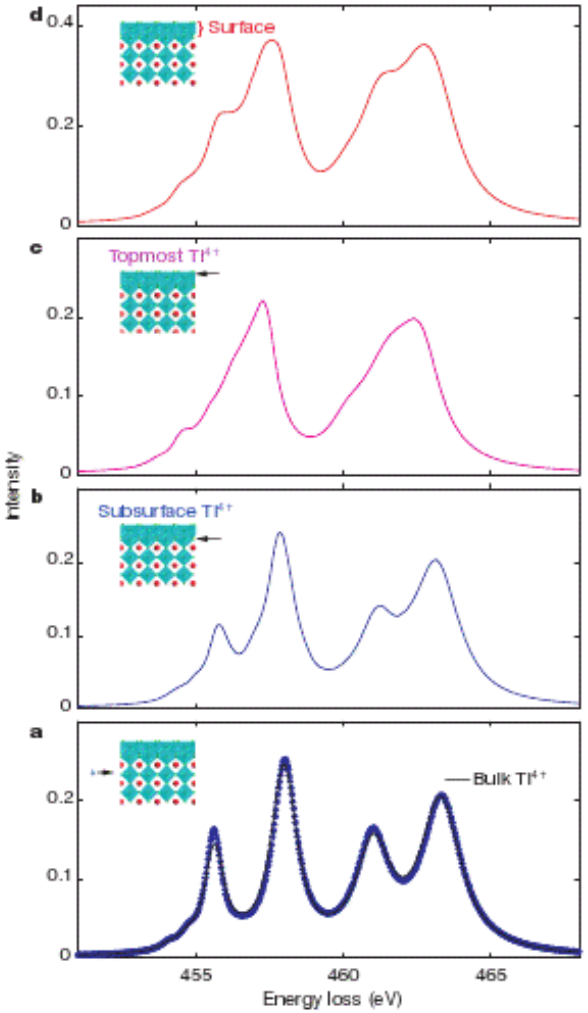
c(4x2)



Zhu, *et al,* Bonding and structure of a reconstructed (001) surface of SrTiO3 from TEM, *Nature* **490,** 384-387 (2012)

c(4x2): EELS





Zhu, *et al,* Bonding and structure of a reconstructed (001) surface of SrTiO3 from TEM, *Nature* **490,** 384-387 (2012)