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# Structural disorder in SrTiO<sub>3</sub> based Ruddlesden-Popper phases

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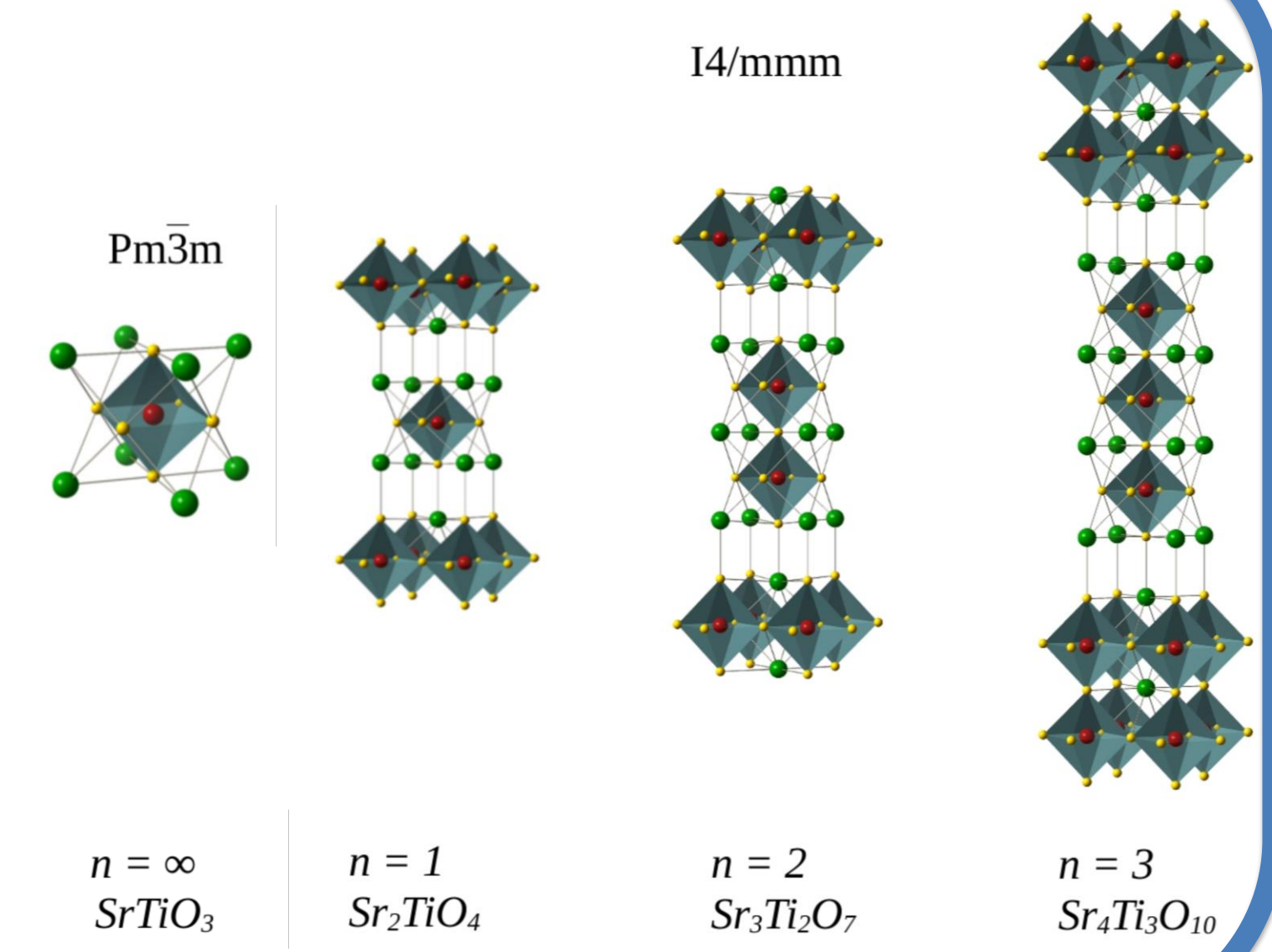
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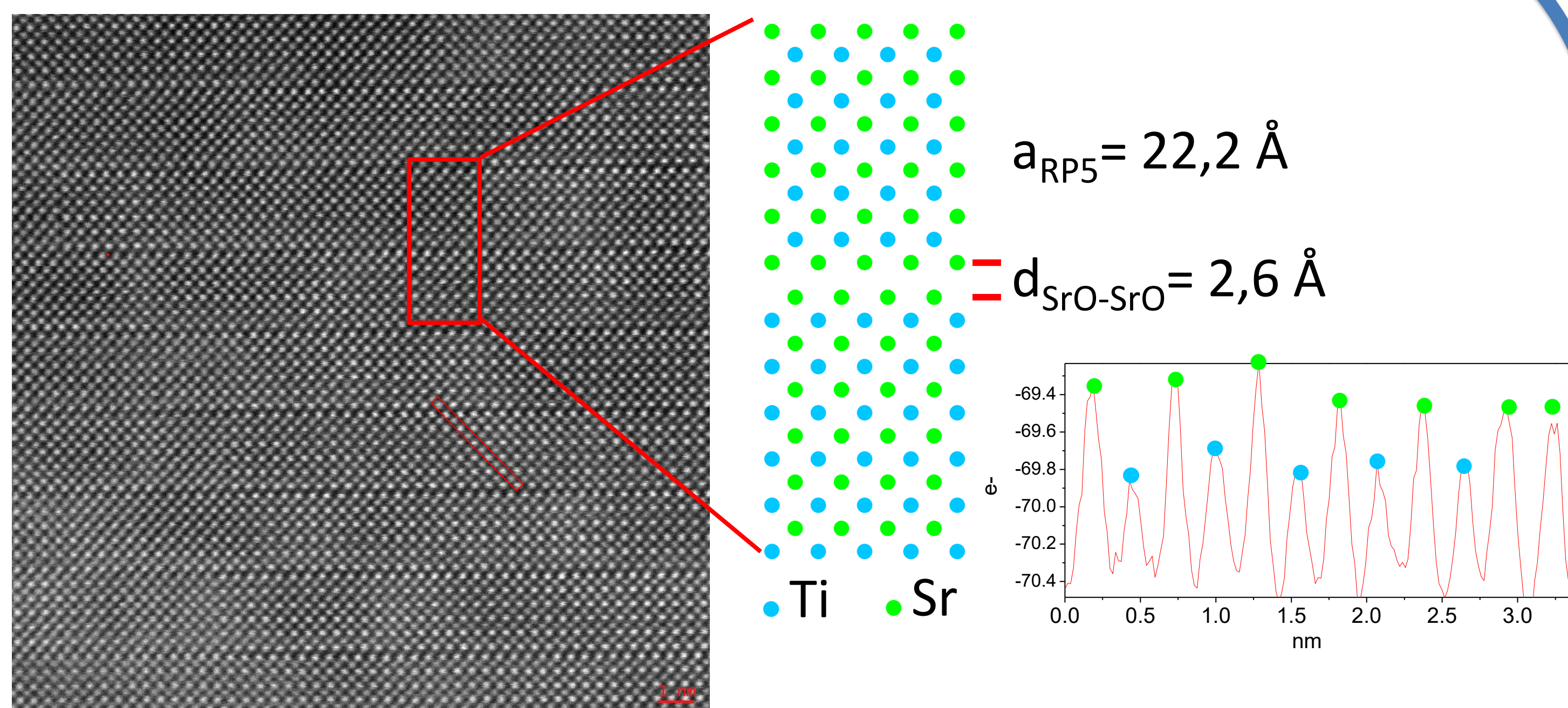
3. GEMaC, UVSQ, CNRS, Université Paris Saclay (France)

## Introduction:

- (SrTiO<sub>3</sub>)<sub>n</sub>(SrO) Ruddlesden-Popper homologous series (RP phases) derive from the STO perovskite structure [1].
- RP phases present outstanding physical properties such as high T<sub>c</sub> superconductivity, colossal magneto-resistance, low loss dielectricity, ferroelectricity, low thermal conductivity for heat harvesting, engineerable optical properties, all of them being tuned by the RP order n [2-4].
- Physical and functional properties strongly correlate to the structural quality, for RP>3 appearance of vertical stacking fault due to the thermodynamic stability
- Toward a better understanding of the vertical stacking fault configurations and impact on the XRD signature.



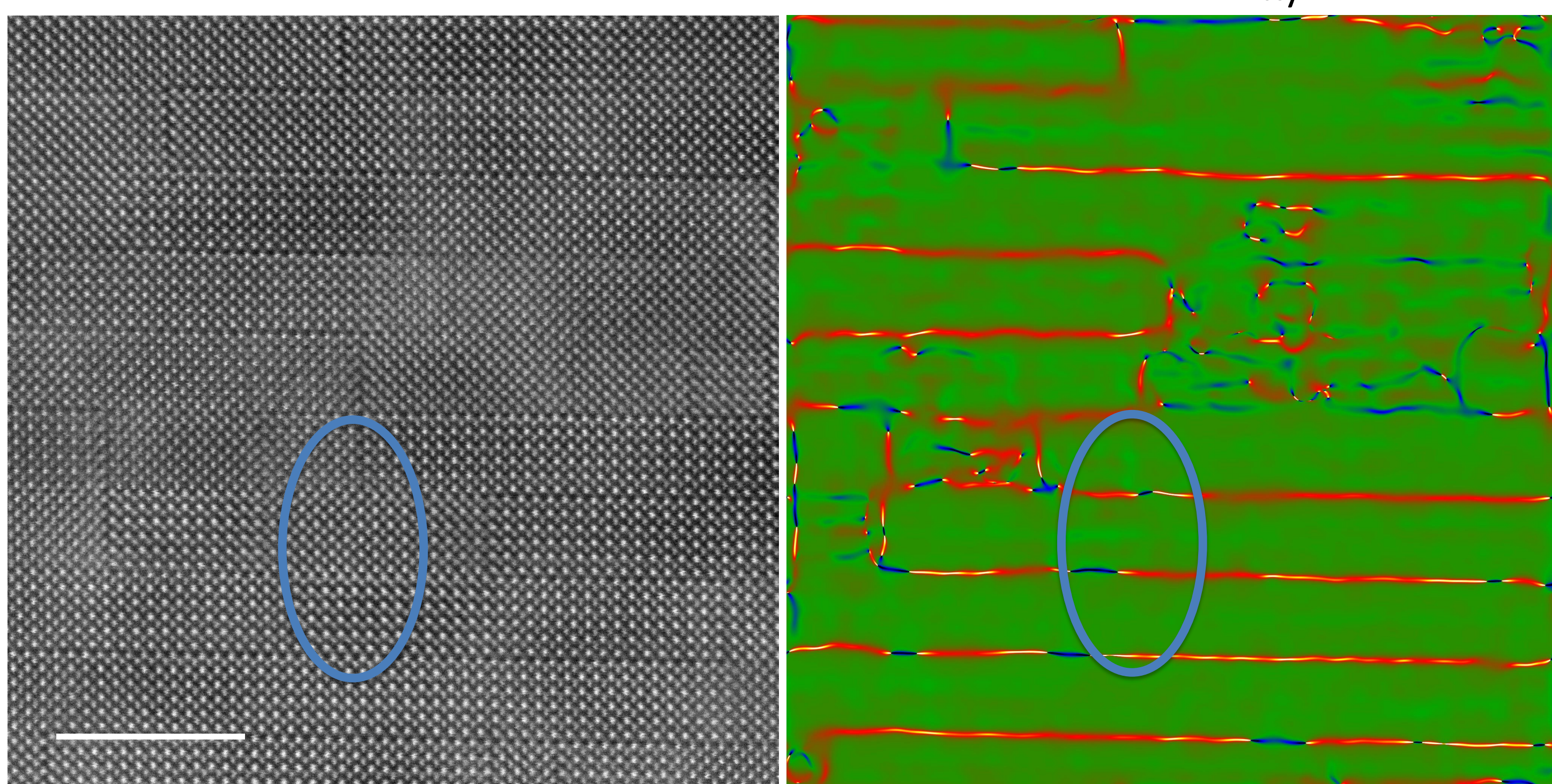
## General RP5 phase TEM characterization:



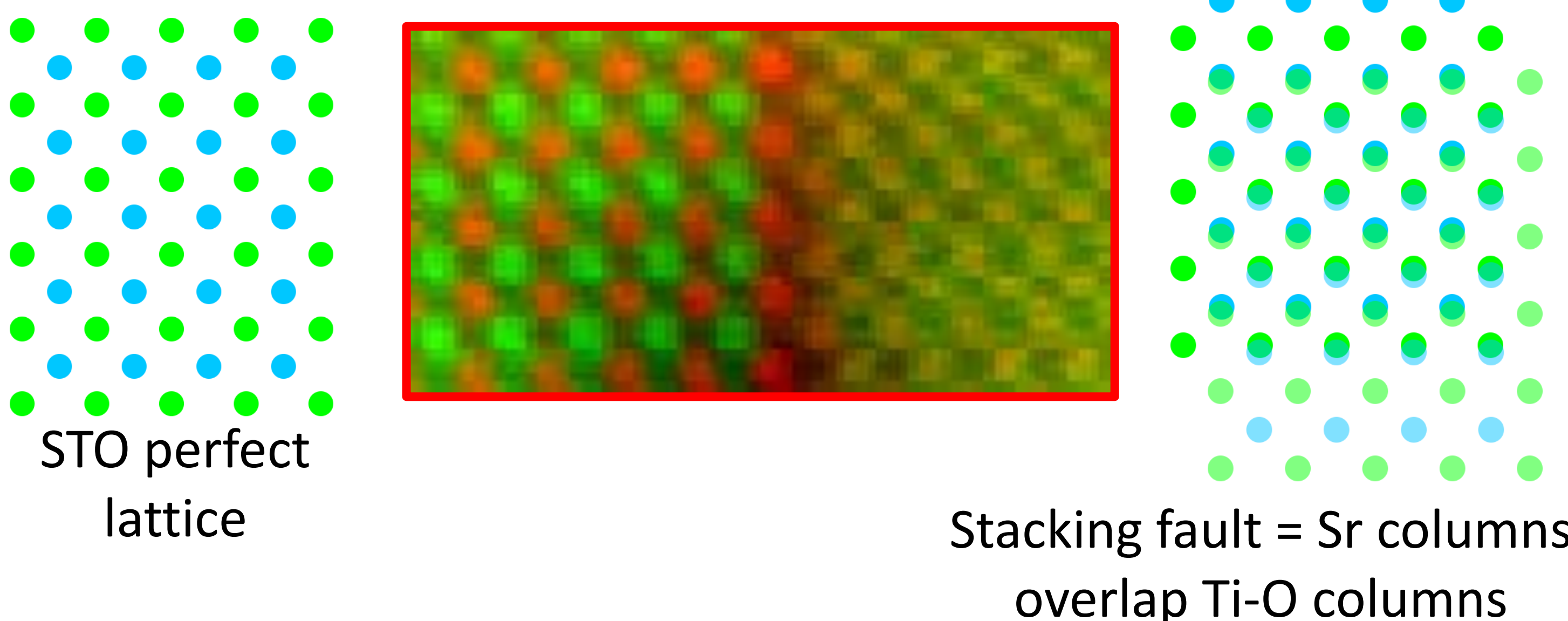
→ Large domains of perfect RP5 Sr<sub>6</sub>Ti<sub>5</sub>O<sub>16</sub>

HRSTEM

GPa map, E<sub>xy</sub>

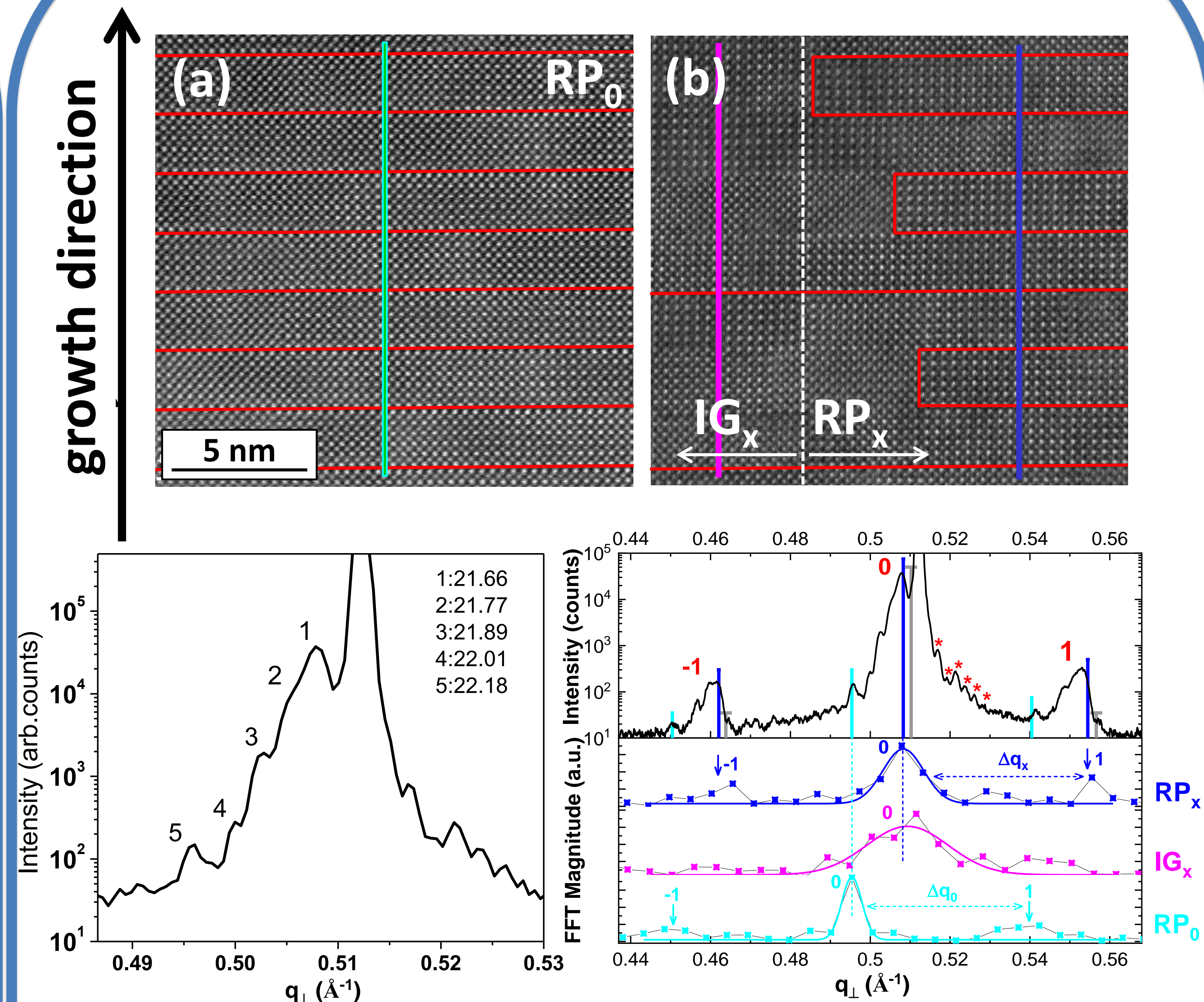


RGB map  
Ti L<sub>2-3</sub> / Sr L<sub>2-3</sub>



→ Several areas with a lot of vertical stacking faults, in all {100} planes involving an overlap of the Sr and Ti-O columns

## Defect consequences on the global structure:



- XRD analyses reveal satellite peaks (no superlattice peaks) corresponding to different RP5 lattice parameters
- From 22,18 Å (perfect RP5) to 21,66 Å due to vertical stacking fault which induce large stress field creating « supercell » with different average lattice parameters

## Conclusion:

- Stoichiometry deviation during MBE growth leads to several vertical stacking fault in all {100} planes
- Those induce “supercell lattice” which modulates the period of the RP5, correlated to satellite peaks on XRD diffractogram
- Toward hyperbolic metamaterial: improving stoichiometric control for a better optimization of optical properties (OFM, EZ-curve, ...)

[1] Christian Ludt *et al.*, Crystals, 11(6), 693 (2011)  
[2] G. A. Pan *et al.*, Nat. Mater. 21, 160 (2022)

[3] Y. Moritomo, *et al.*, Nature 380, 141 (1996)  
[4] N. M. Dawley *et al.*, Nat. Mater. 19, 176 (2020)