Influence of structural distortions on the magnetic order of rare-earth titanates

A. Najev[1, 2] , S. Hameed[2] , D. Gautreau[2, 3] , Z. Wang[2] , J. Joe[2] , M. Pozek[1] , T. Birol[3] , R. M. Fernandes[2] , M. Greven[2] and D. Pelc[1,2]

[1]Department of Physics, Faculty of Science, University of Zagreb, Bijenicka 32, HR-10000 Zagreb, Croatia

[2]School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455, U.S.A.

[3]Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455, U.S.A.

hrzz Croatian Science Foundation

CQM

Acknowledgments and Financing

- Department of Energy, University of Minnesota Center for Quantum Materials, under DE-SC0016371

- Croatian Science Foundation, Project IP-01-2018-2970

Transition Metal Oxides – Perovskite Structure

- Transition metal oxides: Nickelates, Manganites, Cobaltates, Titanates, Ruthenates, Cuprates, Vanadates,…
- Unpaired *d* orbital electrons
- Variety of low symmetry structural distortion
- Wide scope of different properties:

  High Tc superconductivity, Colossal Magnetoresistance, CDW, SDW,

  Ferroic and Multiferroic behaviour, Metal-insulator transitions, …
- Mott insulators, Charge transfer insulators, Metals
- Coupling of spin, charge, orbital and structural degrees of freedom

Transition Metal Oxides – Perovskite Structure

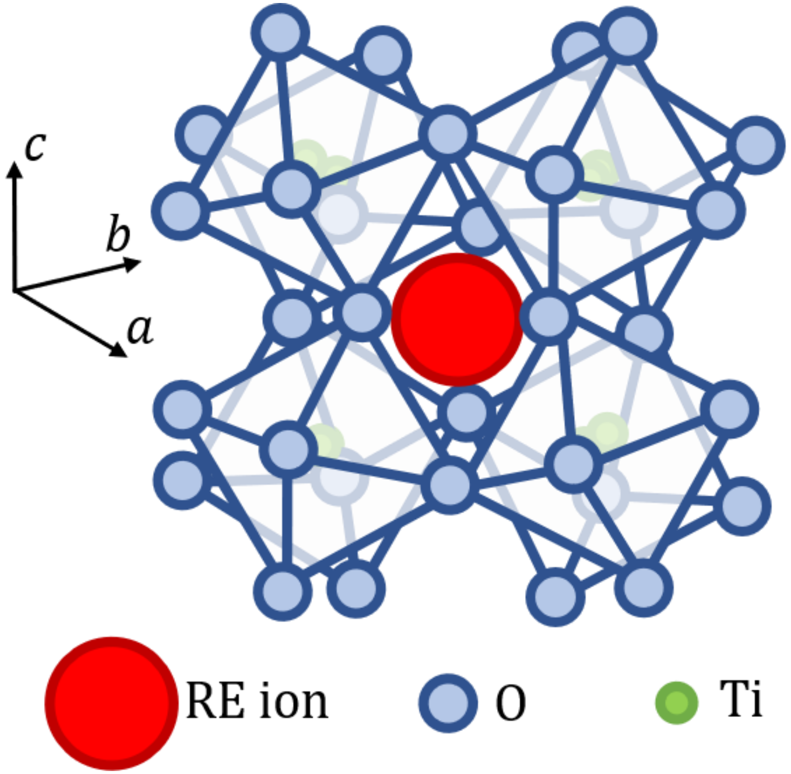
- Transition metal oxides: Nickelates, Manganites, Cobaltates, Titanates, Ruthenates, Cuprates, Vanadates,…
- Unpaired *d* orbital electrons
- Variety of low symmetry structural distortion
- Wide scope of different properties:

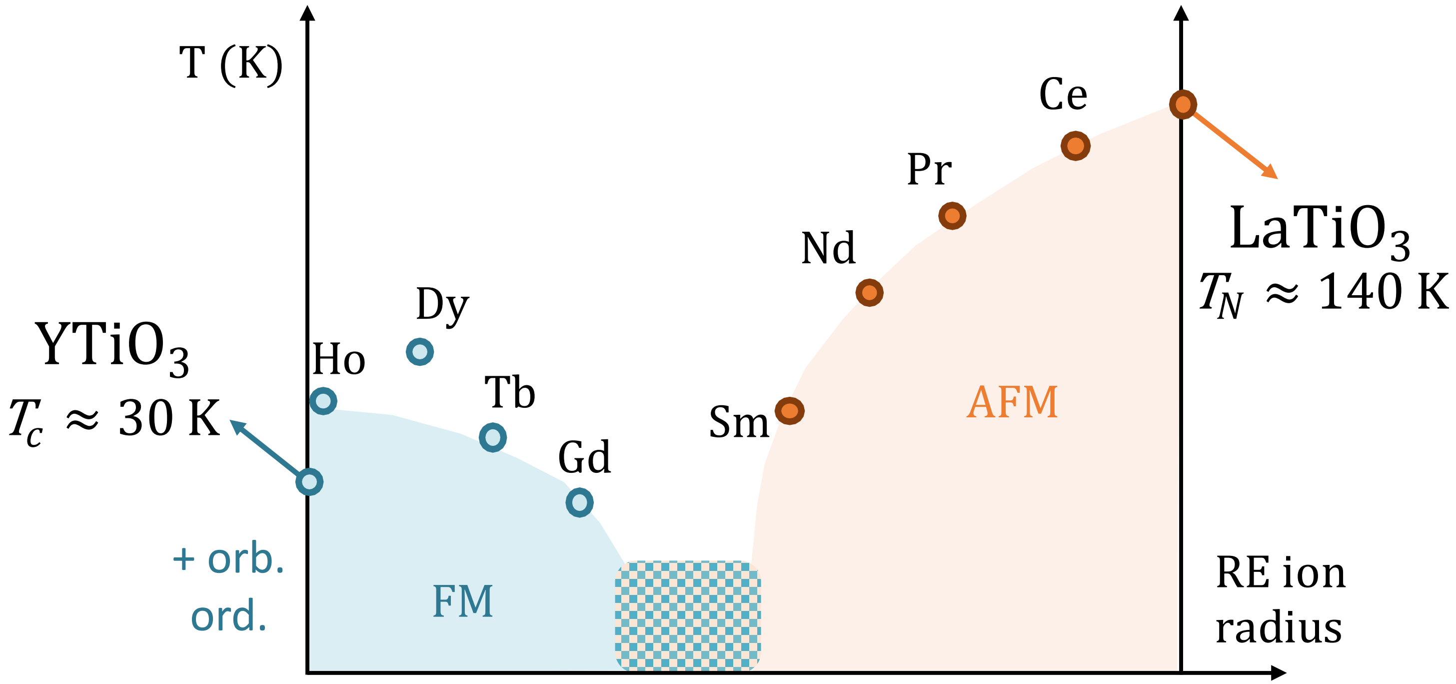
  High Tc superconductivity, Colossal Magnetoresistance, CDW, SDW,

  Ferroic and Multiferroic behaviour, Metal-insulator transitions, …
- Mott insulators, Charge transfer insulators, Metals
- Coupling of spin, charge, orbital and structural degrees of freedom

Rare-earth Titanates

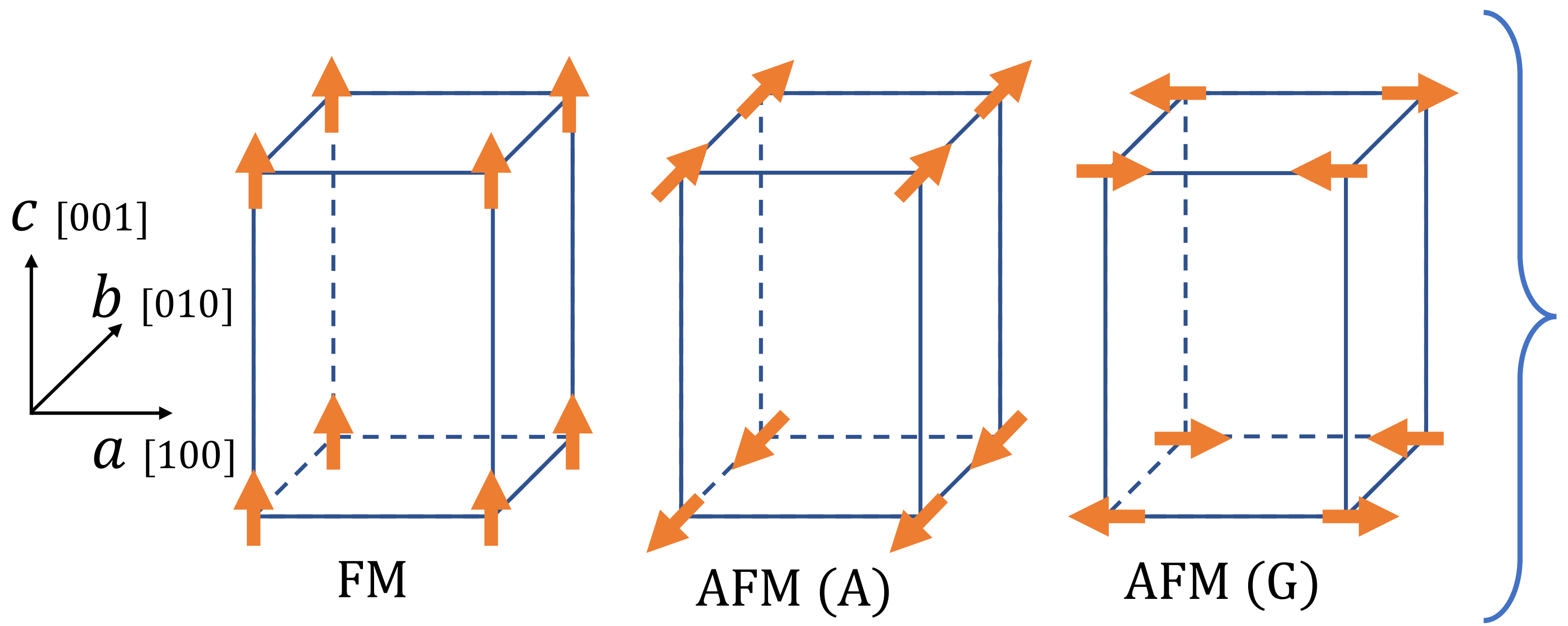
- Model three-dimensional electron-correlated system of doping controlled bandwidth and band filling
- Mott-Hubbard insulators with FM and AFM magnetic groundstate





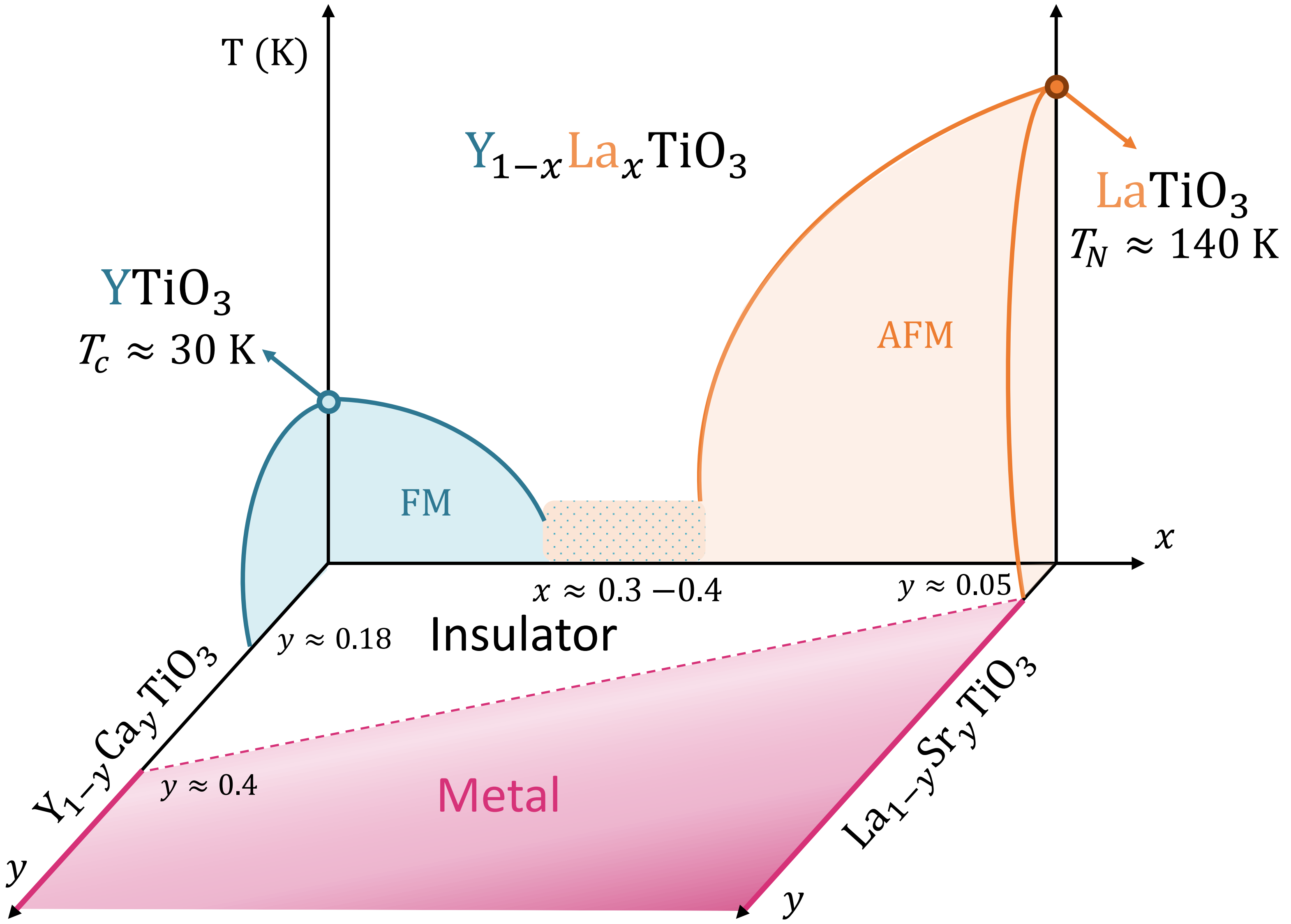
Rare-earth Titanates

- Pbnm orthorombic space group
- Additional octahedral distortions without symmetry breaking
- Superexchange sensitive to low symmetry structural distortions

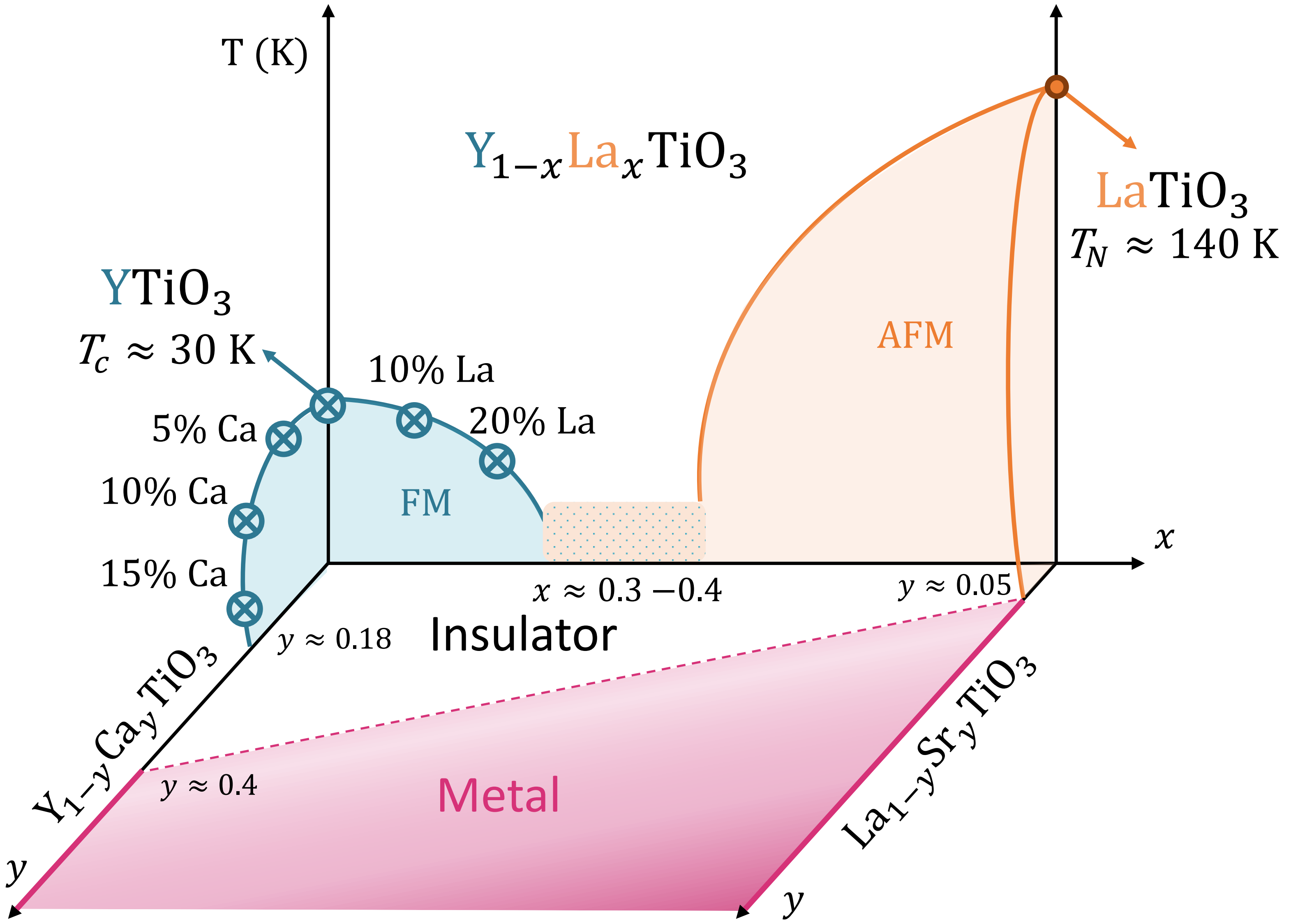


Superposition of different spin orders within the same magnetic symmetry

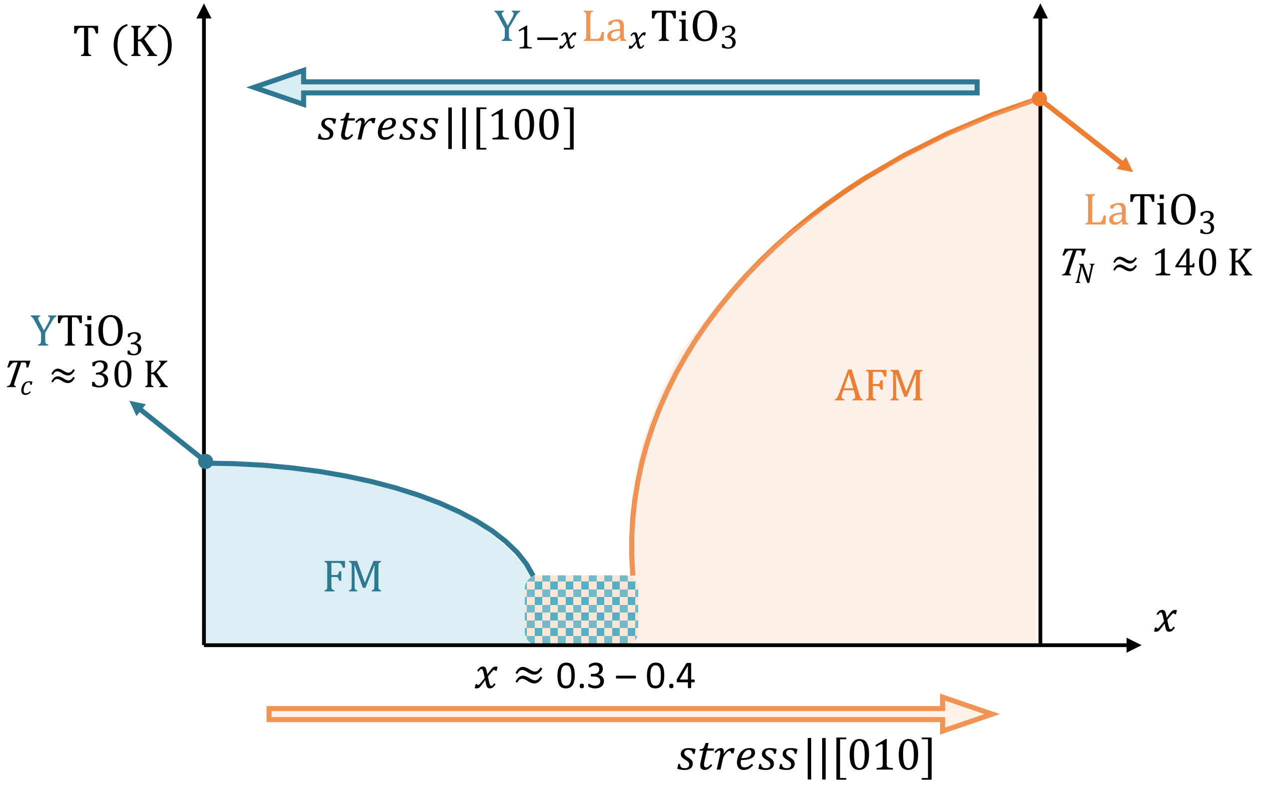
Rare-earth Titanates



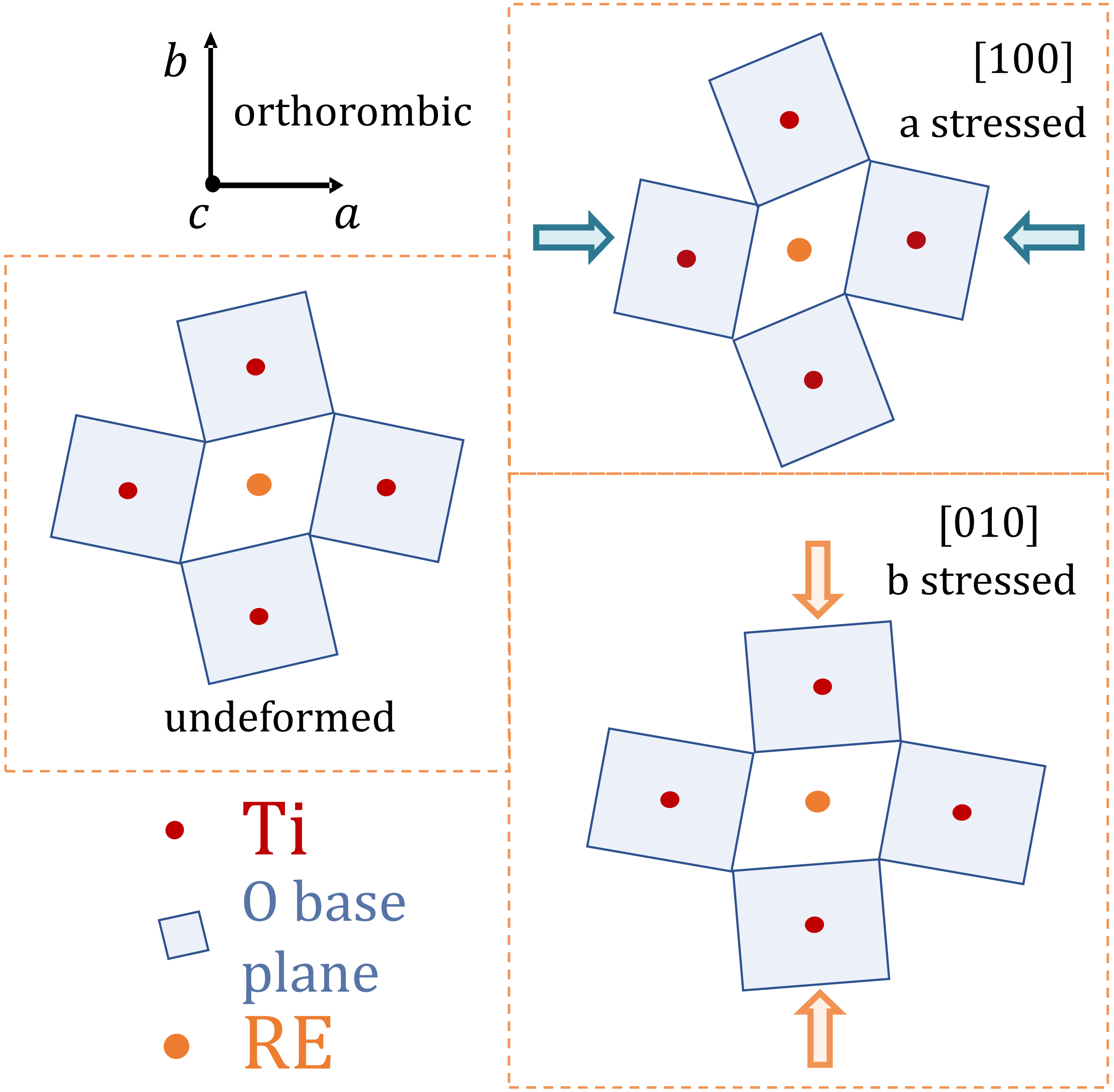
Rare-earth Titanates



Effect of Uniaxial Stress on the FM Order - Theory



W. Knafo et al., Phys. Rev. B (2009) **79**, 054431



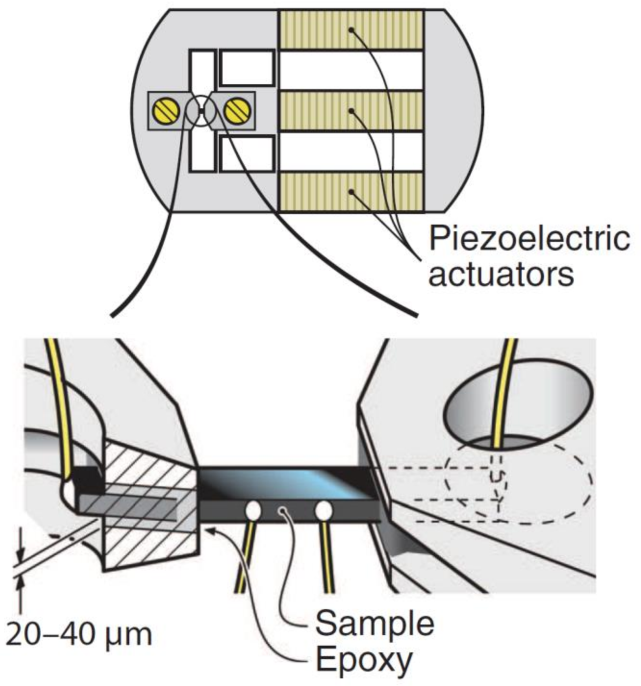
Uniaxial Stress Experiments

- proximity to a structural and electronic instability
- strain-induced lowering of the structural symmetry

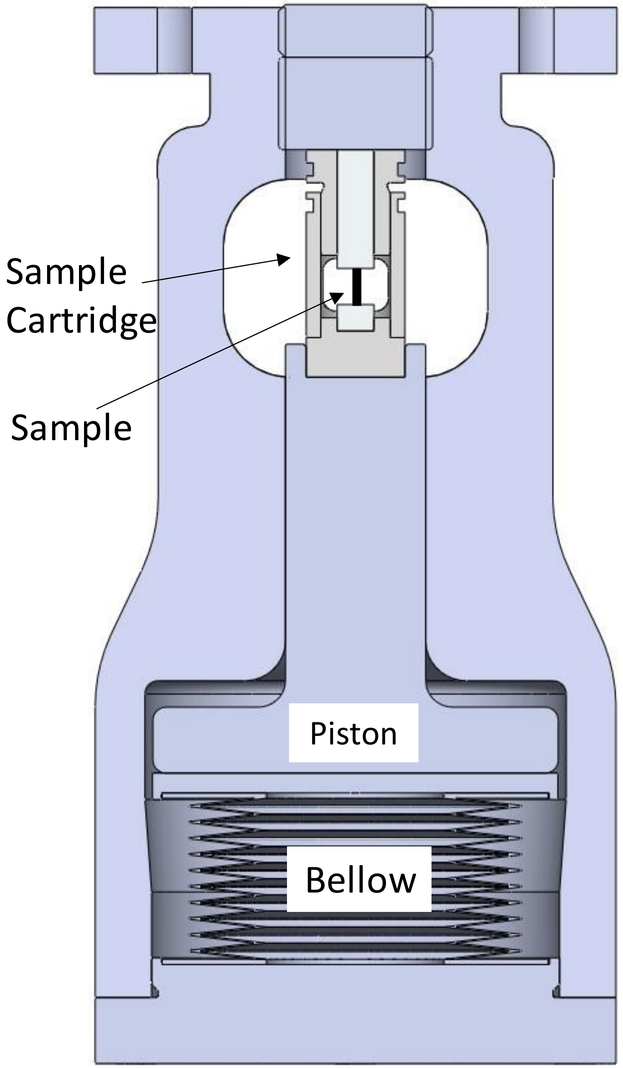
Kim *et al.*, Science (2018) 362, 1040 strain-tuning the CDW in high-temperature superconductors

Steppke *et al.*, Science (2017) 355, eaaf9398 uniaxial pressure manipulation of superconductivity in strontium ruthenate

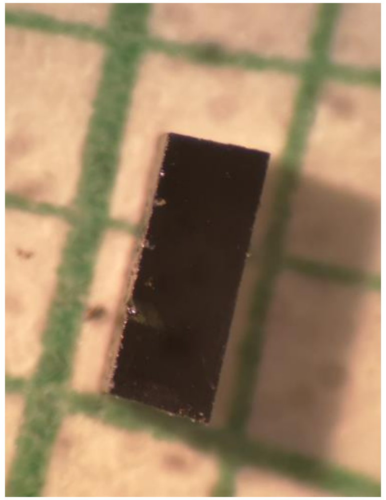
Aetukuri *et al.*, Nature Physics (2013) 9, 661 epitaxial strain control of metal-insulator transitions in vanadium oxides



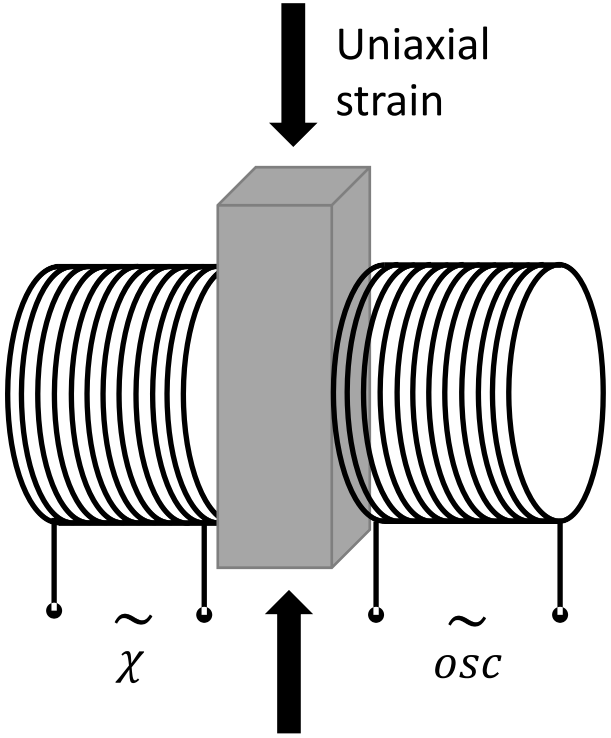
Custom Made Cell for Uniaxial Stress



- Continuous pneumatic *in situ* control of sample stress
- LVT stress-strain diagrams

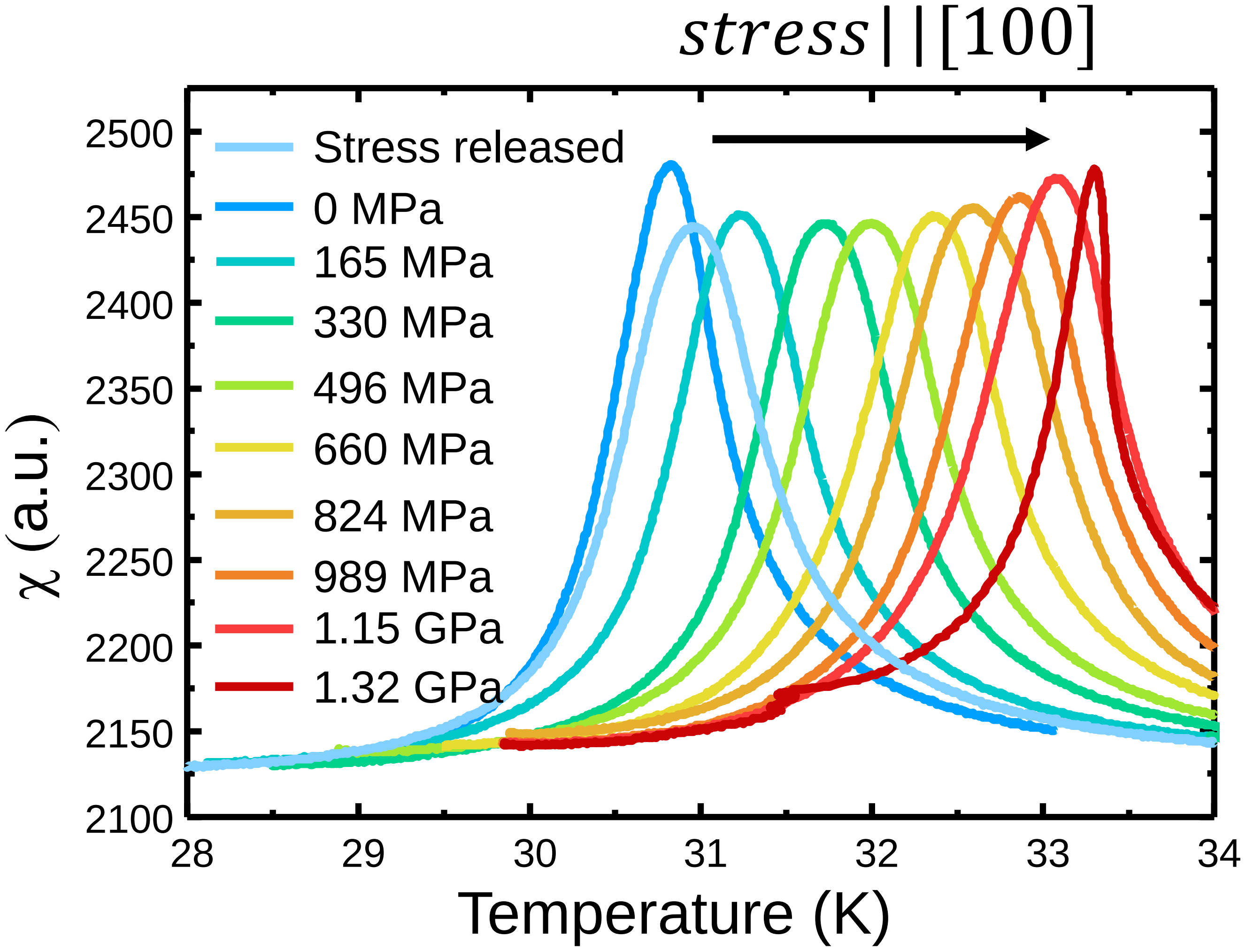


Polished single crystals

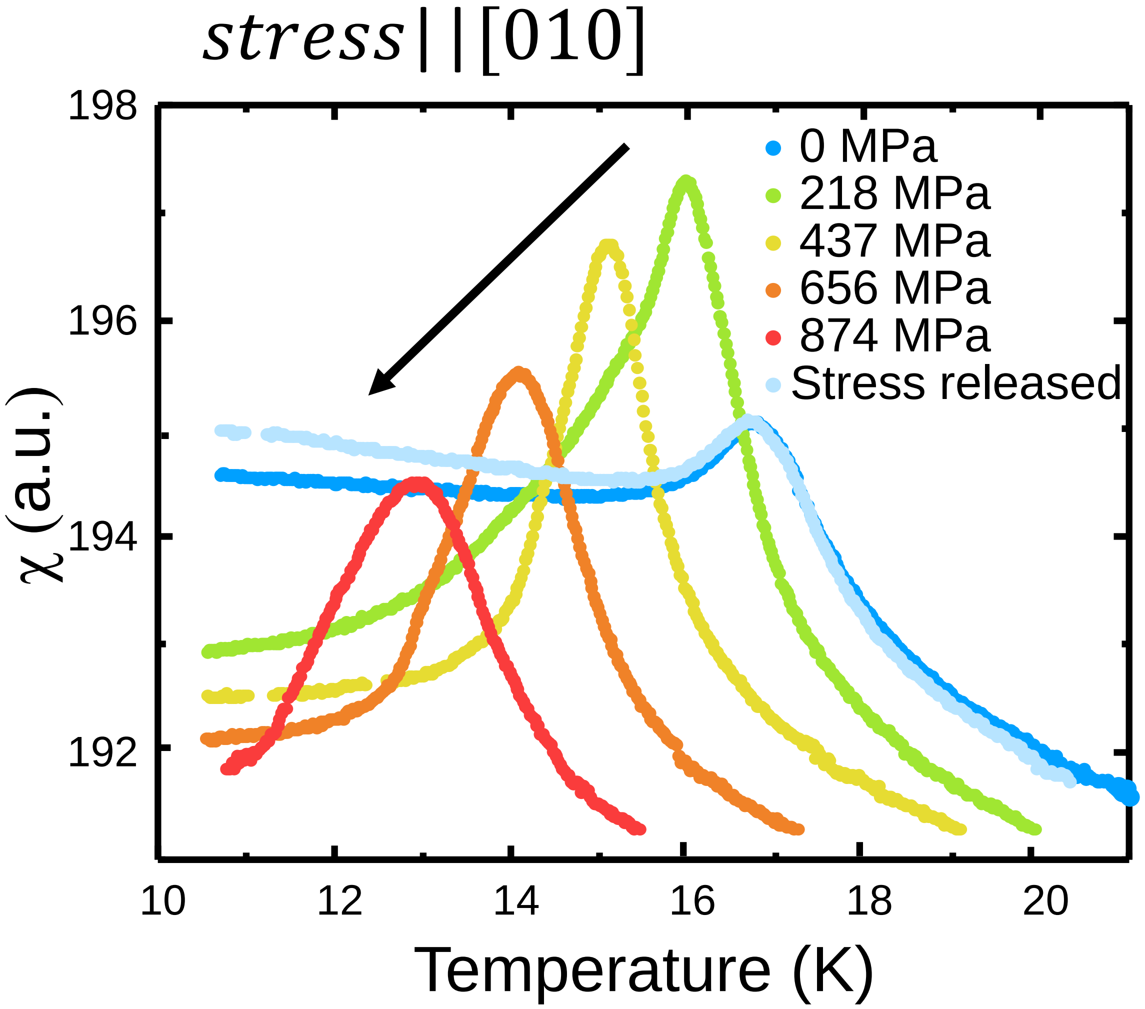


Measurement setup

Uniaxial Stress Control of FM Order Temperature



$YTiO_3$

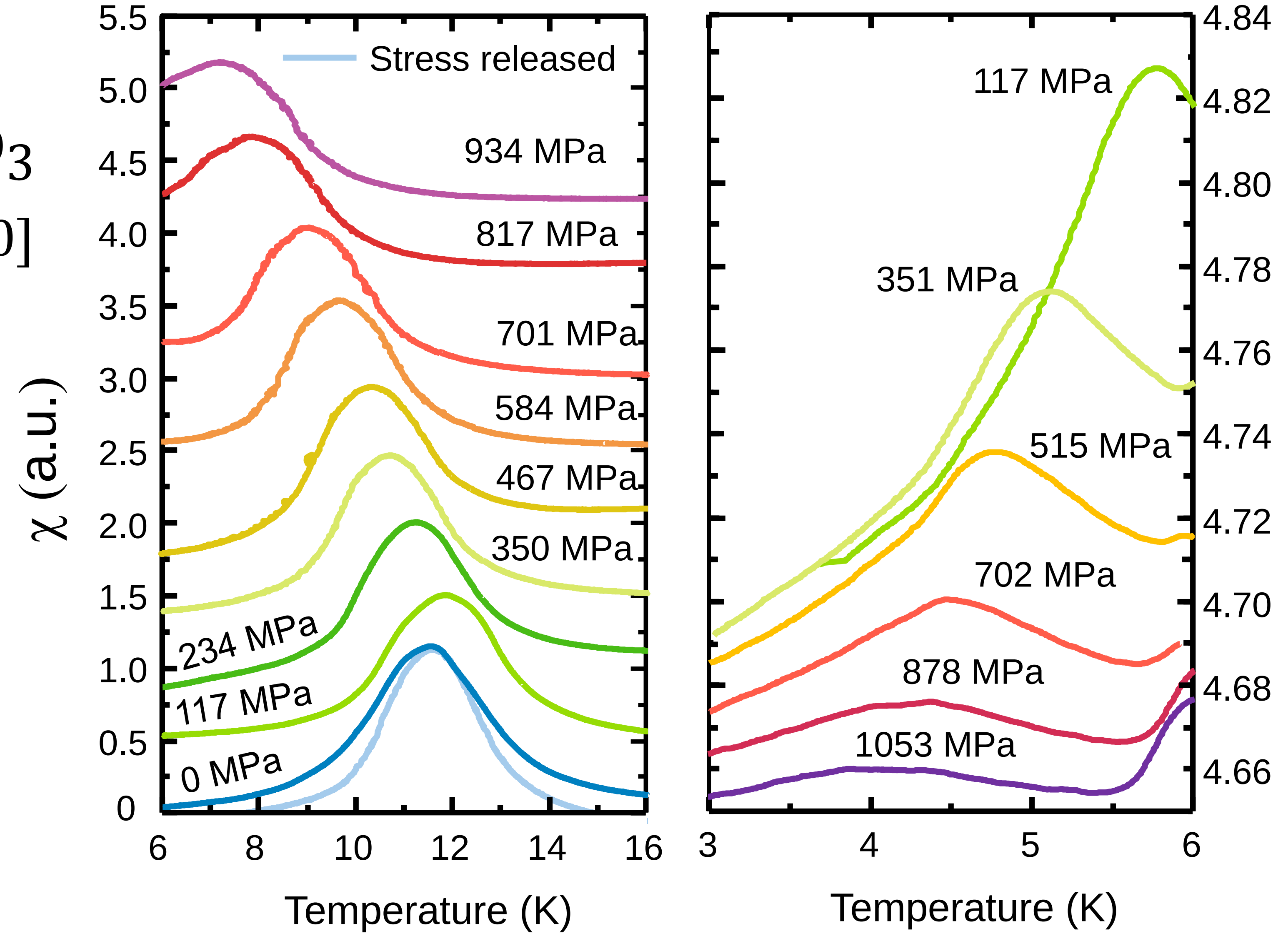


$Y_{0.9}La_{0.1}TiO_3$

Uniaxial Stress Control of FM Order Temperature

$Y_{0.9}Ca_{0.1}TiO_3$

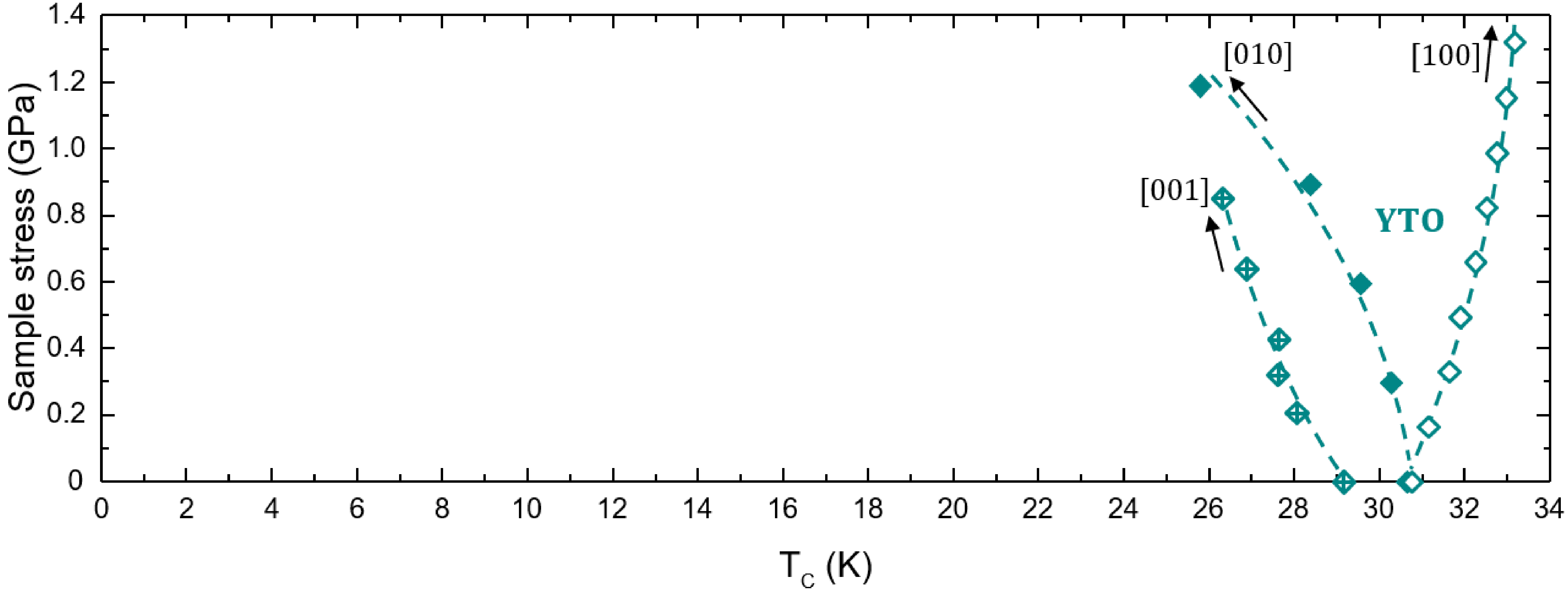
stress||[010]



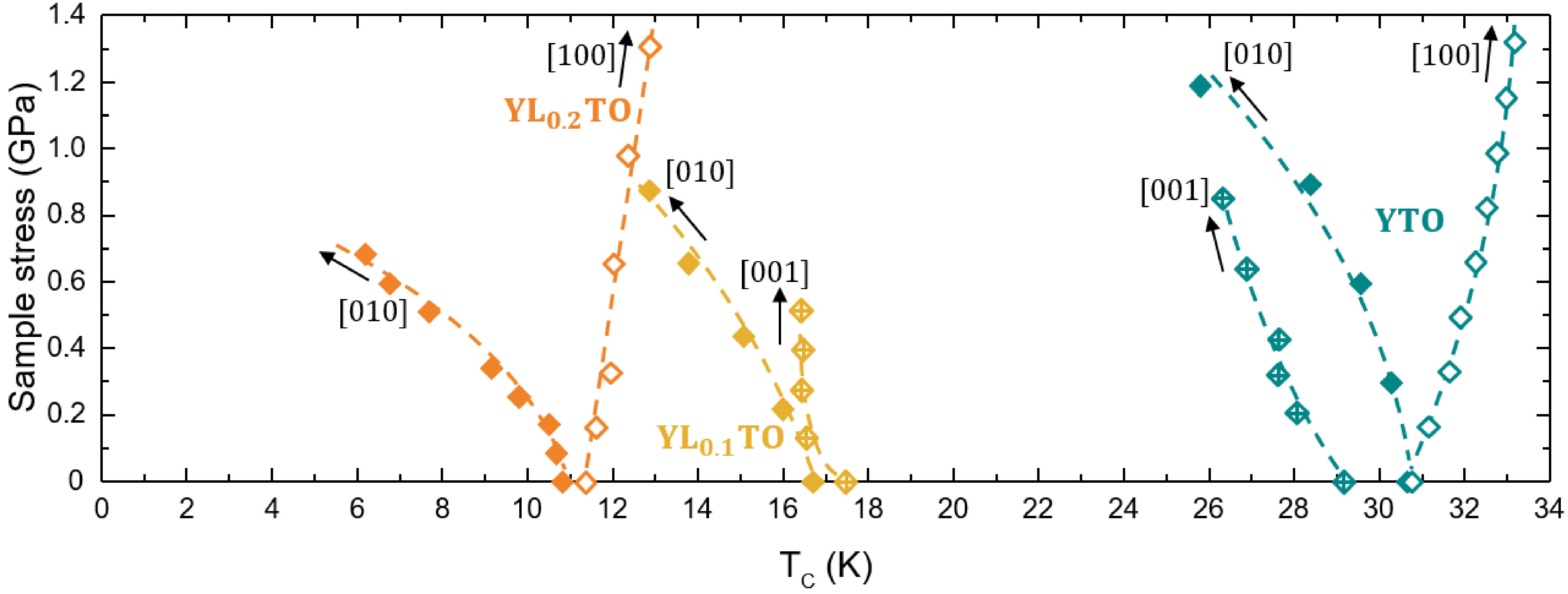
$Y_{0.85}Ca_{0.15}TiO_3$

stress||[010]

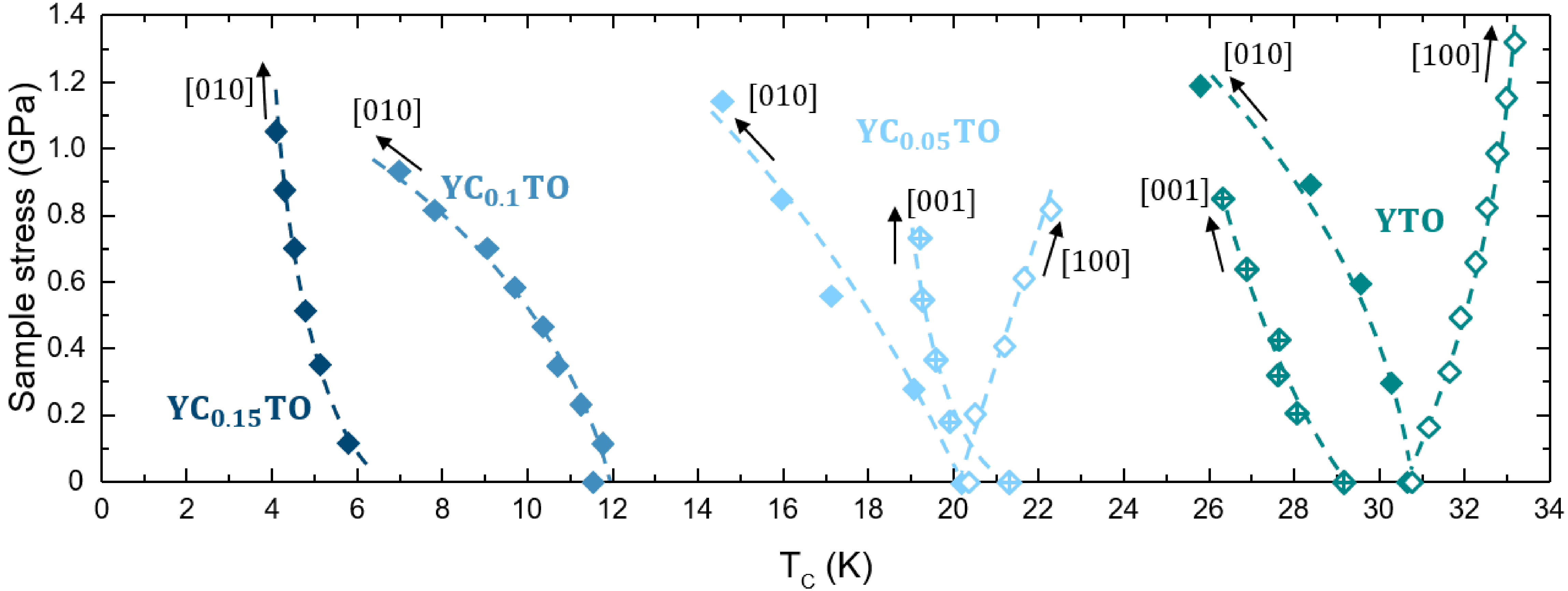
Phase Diagram of Stressed RE Titanates



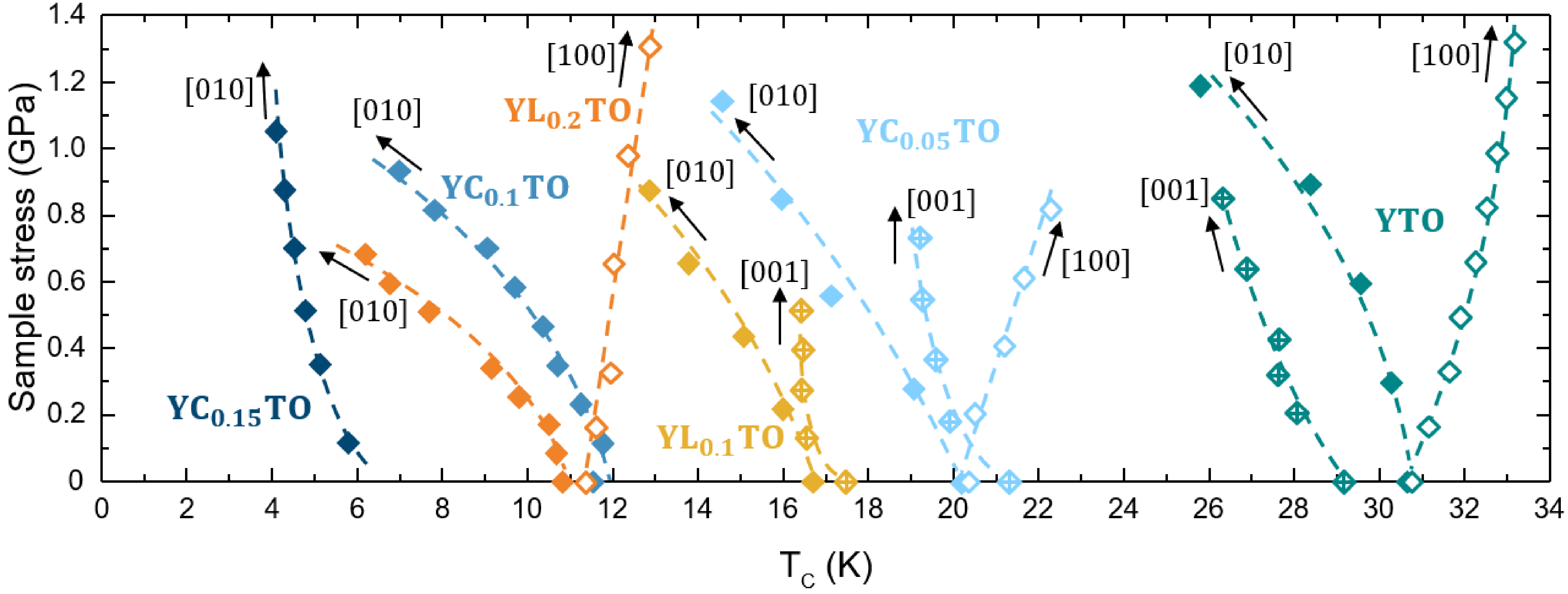
Phase Diagram of Stressed RE Titanates



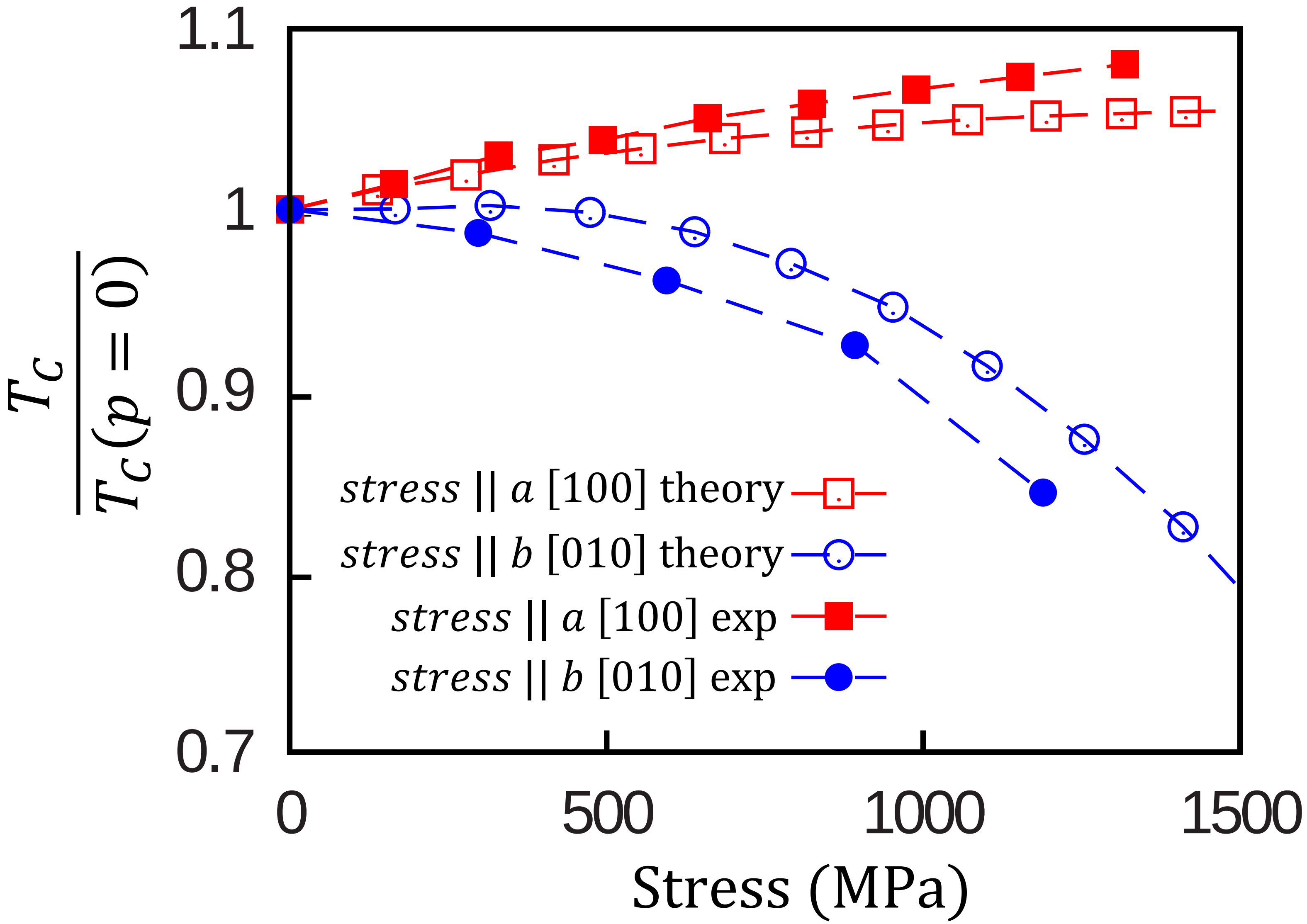
Phase Diagram of Stressed RE Titanates



Phase Diagram of Stressed RE Titanates



DFT+U Mean Field Calculation for $YTiO_3$



Good agreement between theory and experiment!

Conclusion and Outlook

- Unique pressure cell for high and homogenous uniaxial stress experiments
- No QCP in the doped compounds, FM-PM is a first order transition
- Experiment trends well captured by theory
- Similarity of chemical doping and uniaxial strain?
- Importance of low symmetry structural distortions in elucidating the physics of complex oxides

CQM
hrzz
Croatian Science Foundation

Thank you!