Karlsruher Institut für Technologie

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Doping-Regulated Room-temperature Dislocation Plasticity in Oxides: A scale bridging study on $SrTiO_3$

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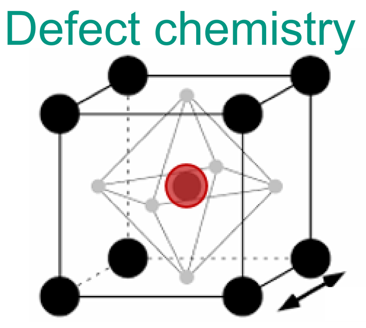
Background & Motivation

Modern functional oxides are mainly tailored by doping, involving the study of point defects and their interactions in the solid state. Recently, dislocations have been shown to enhance the mechanical and functional properties of advanced oxides [1], benefiting potential applications such as in actuators and sensors. This necessitates understanding the interaction of dislocations and point defects in functional oxides.

Objective: Identify the mechanism controlling dislocation-mediated plasticity across the length scale on single-crystal $SrTiO_3$ by defect chemistry engineering.

Defect chemistry of $SrTiO_3$



Oxygen exchange equilibrium reaction;

$O_O^x \underset{reduction}{\rightleftharpoons} V_O^{\cdot\cdot} + 2e' + \frac{1}{2}O_2(g)$

$V_O^{\cdot\cdot} + \frac{1}{2}O_2(g) \underset{oxidation}{\rightleftharpoons} O_O^x + 2h^{\cdot}$

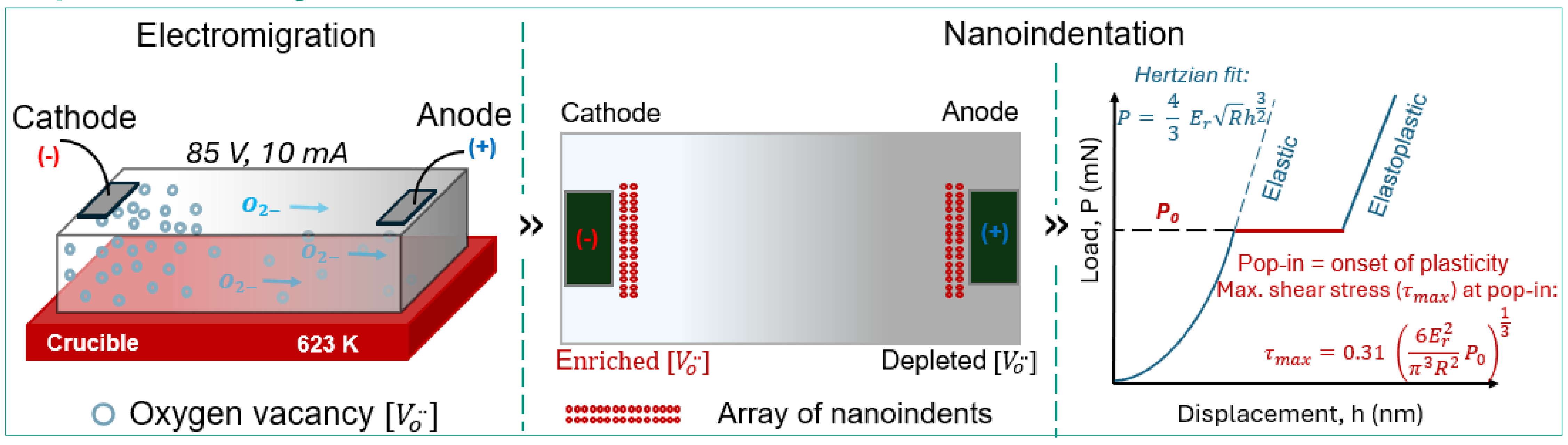
Donor doping (e.g. Nb^{5+} substitute Ti^{4+})

$Sr_{Sr}^x + O_O^x = V_{Sr}'' + V_O^{\cdot\cdot} + SrO(s)$

Excess electrons are compensated by V_{Sr}''

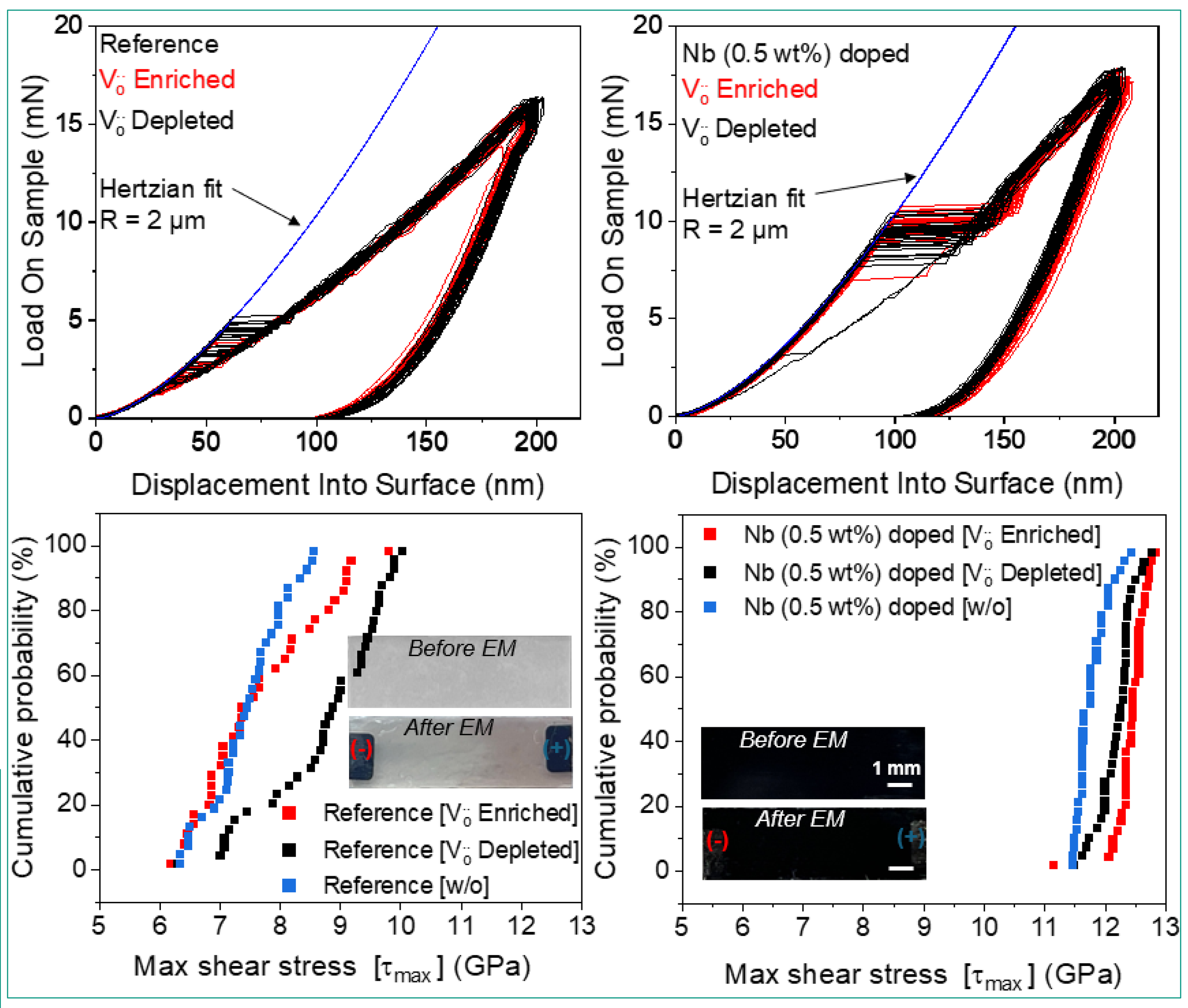
NANO/MICROSCALE Electromigration(EM) & Nanoindentation

Experiment design



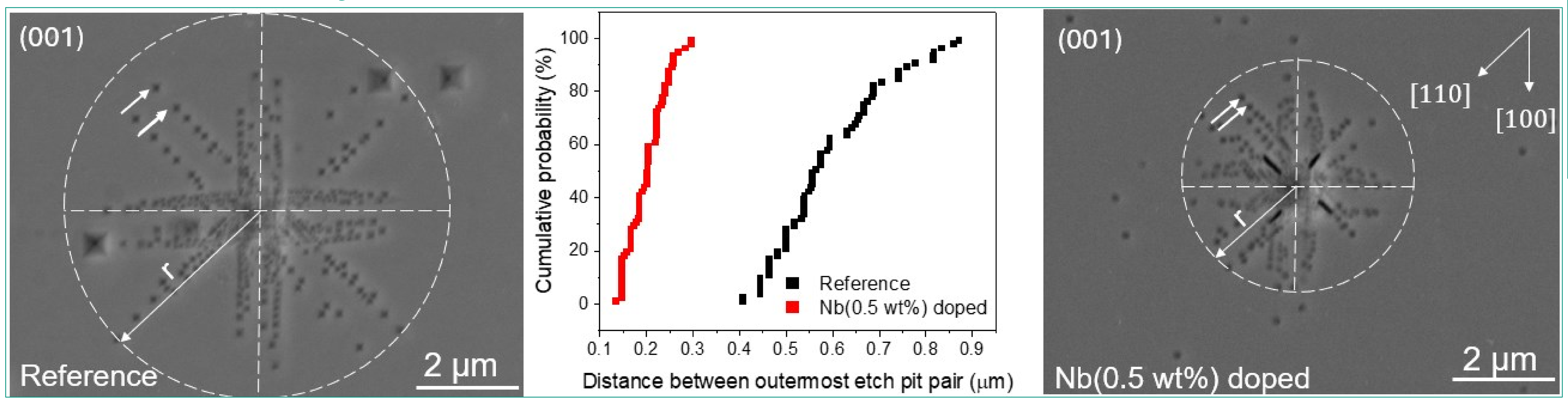
Electromigration tuning $V_O^{\cdot\cdot}$ concentration with corresponding electrocoloration [2] | Dislocation nucleation and mobility studies using 2 µm indenter tip radius and a strain rate of 0.05/s

Dislocation nucleation



- Reference:
  - Cathode: lower τ_{max} at pop-in.
  - Anode: relatively higher τ_{max} at pop-in event
- Nb (0.5 wt%) doped:
  - No electromigration, τ_{max} at pop-in event overlaps.
  - Blue plots: before electromigration.

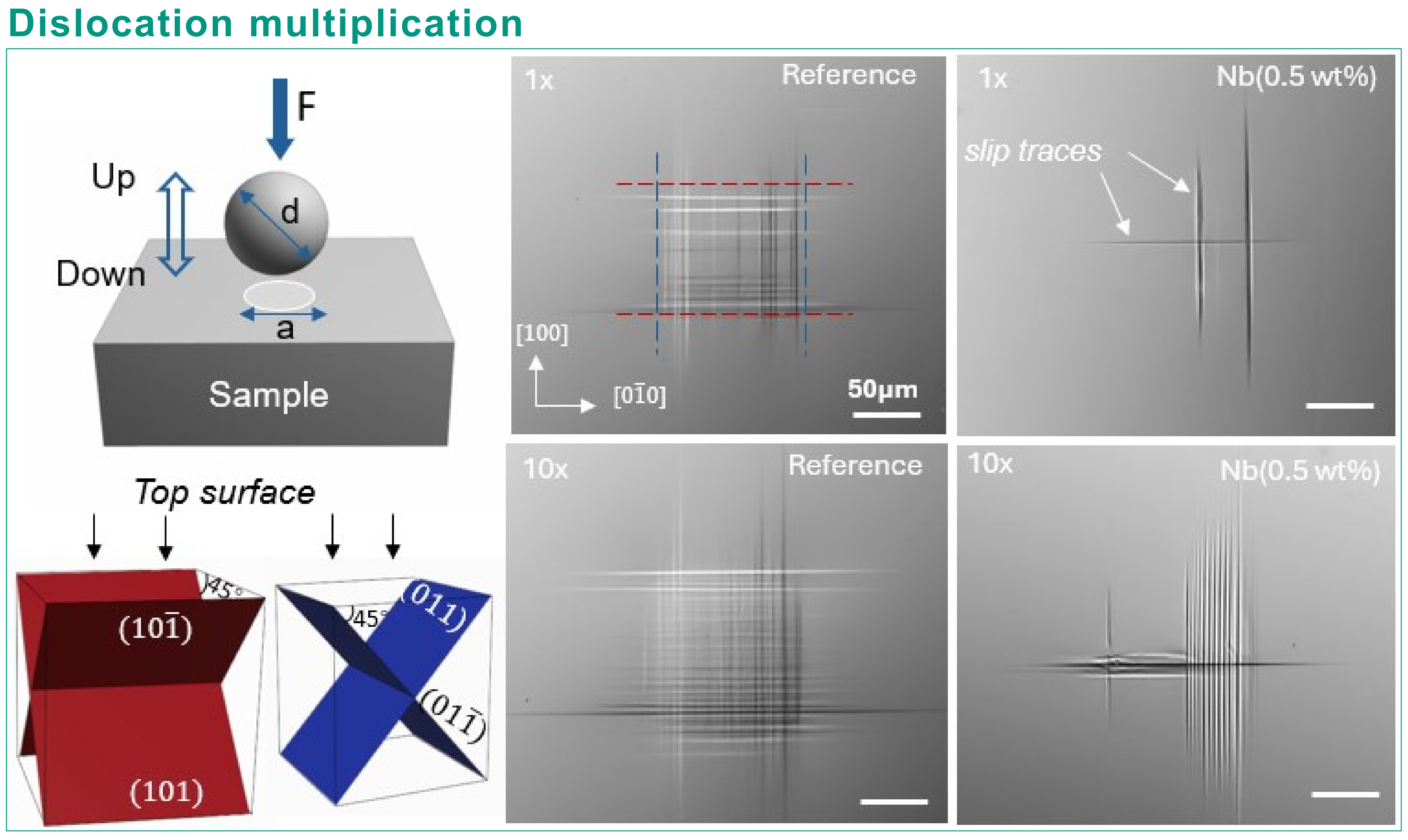
Dislocation mobility



Lattice friction stress [3] estimation: $\tau_f = \tau_a + \tau_d + \tau_{im}$ | $\tau_{f(reference)} = 77 \pm 6\ MPa$, $\tau_{f(Nb(0.5\ wt\%)doped)} = 93 \pm 29\ MPa$

MESOSCALE Cyclic Brinell indentation

Dislocation multiplication



- Cyclic Brinell indentation with a steel ball (d=2.5 mm) and 1.5 kgf (F) [4].
- 1x and 10x represents the number of indentation cycles (10x for 10 cycles).
- Discrete density of slip traces for Nb(0.5 wt%) doped $SrTiO_3$ even after 10x Brinell indentation cycles

Discussion

- $V_O^{\cdot\cdot}$ promotes dislocation nucleation during nanoindentation coupled with electromigration
- Not only nucleation but also dislocation mobility is hindered by Nb doping.
- Lattice friction stress hindering dislocation mobility is ≈ 32% higher for Nb(0.5 wt%) doped.

Summary

- Dislocation nucleation, multiplication, and mobility across the length scales
- Room-temperature dislocation-based plasticity altered by point defect engineering from nano/microscale to mesoscale and macroscale
- $V_O^{\cdot\cdot}$ identified as defect species which promotes dislocation nucleation
- Defect chemistry engineering as a potential tool to identify more RT deformable ceramics

Outlook

- **MACROSCALE test: uniaxial bulk compression**
- Acceptor and donor doping on A-site and the effect of temperature

References

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[4] Okafor, C., et al. (2022). J. Am. Ceram. Soc. 105(4): 2399-2402.

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