Oxygen partial pressure dependence of Power factor in SrTiO$_3$ ceramics: Are thermoelectric oxides "stable in air"?

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505-284-9711

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Sandia National Laboratories

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Non-oxide thermoelectrics "unstable in air"

n-Type zT

p-Type zT

Snyder, Toberer Nat. Mat. 08

P-type

N-type

(a)

Ca$_3$Co$_4$O$_9$
— d) crystal
— e) ceramic
— f) ceramic

Bi$_2$Sr$_2$Co$_2$O$_x$
— g) crystal

Na$_x$CoO$_2$
— a) crystal
— b) ceramic
— c) ceramic

(b)

h) (Zn,Al)O
— i) (In,Ge)$_2$O$_3$
j) Sr(Ti,Nb)O$_3$
— k) (Ca,Yb)MnO$_3$
— l) (Sr,Ba)PbO$_3$

zT

Temperature (K)

Terasaki APL Mat. 16
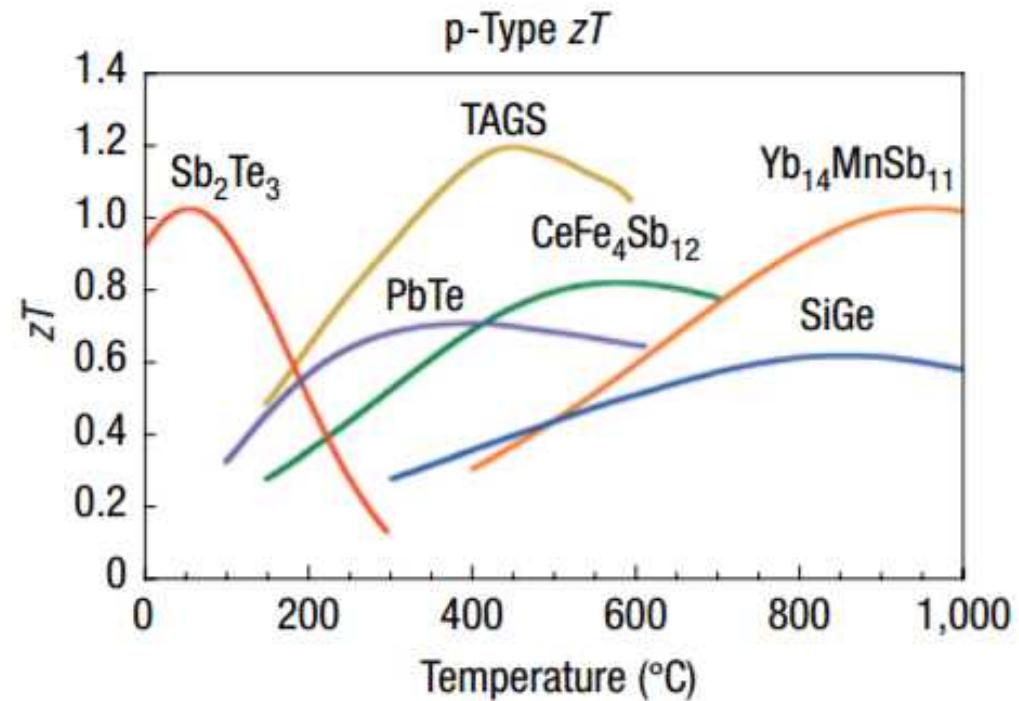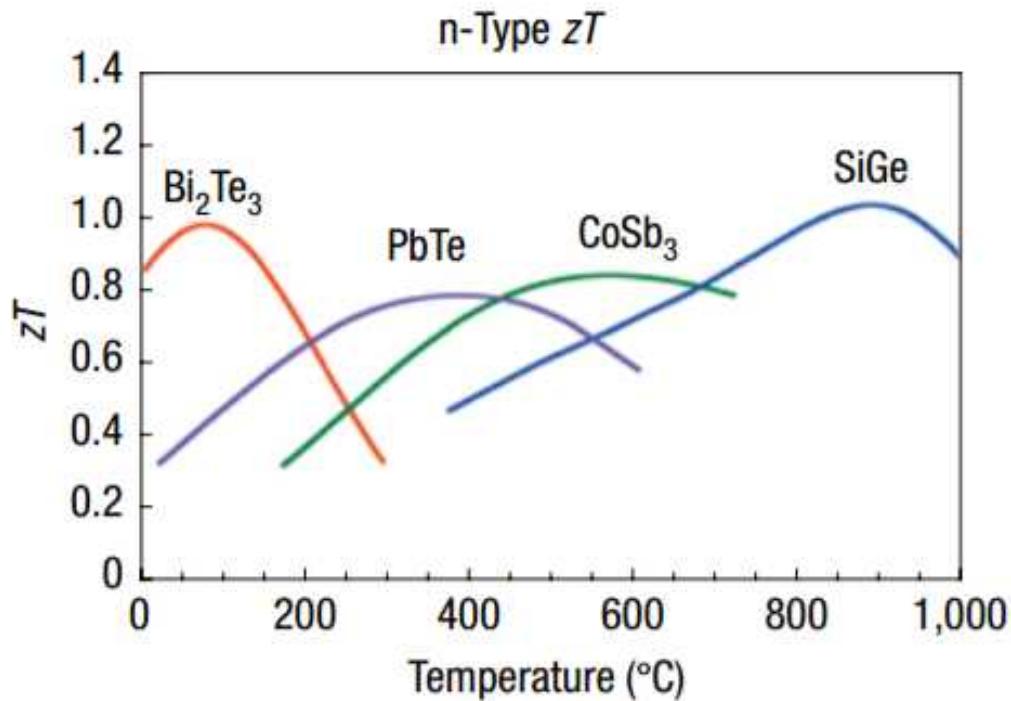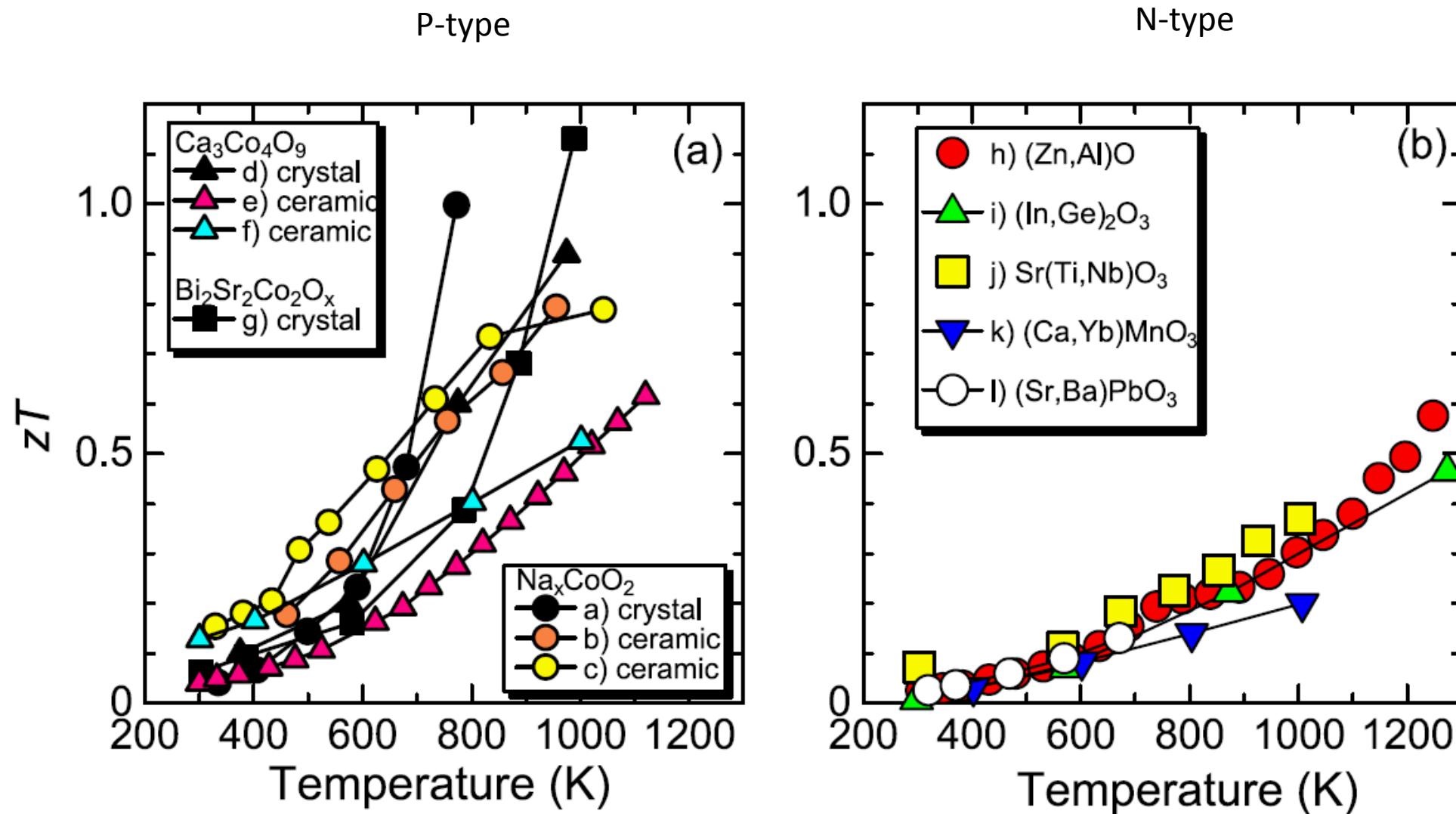
Thermoelectric oxides for high temperature power generation:

-large band gaps
-high melting points
-large materials discovery space
-established ceramic processing
-cheap
-Stable operation in air

Table 1. Power generation characteristics of present oxide modules as compared with the others reported.

Reference	Materials	No. of p–n	Jointing technique	T_{hot} (K)	ΔT (K)	V_0 (V)	P_{max} (mW)	Legs size (mm)	Power density (mW cm^{-2})
Urata et al [61]	p-Ca$_{2.7}$Bi$_{0.3}$Co$_4$O$_9$ n-CaMn$_{0.98}$Mo$_{0.02}$O$_3$	8	Ag	1273	298	1.0	170	5 × 5	42.5
Souma et al [64]	p-NaCo$_2$O$_4$ n-Zn$_{0.98}$Al$_{0.02}$O	12	Diffusion welding	934	455	0.8	52.5	3 × 4	18.2
Matsubara et al [63]	p-Ca$_{2.75}$Gd$_{0.25}$Co$_4$O$_9$ n-Ca$_{0.92}$La$_{0.08}$MnO$_3$	8	Pt paste	773	390	1.0	63.5	3 × 3	44.1
Souma et al [62]	p-NaCo$_2$O$_4$ n-Zn$_{0.98}$Al$_{0.02}$O	12	Ag, diffusion welding	839	462	0.8	58	3 × 4	20.1
Shin et al [65]	p-Li-doped NiO n-Ba$_{0.2}$Sr$_{0.8}$PbO$_3$	4	Sintering	1164	539	0.4	34.4	3 × 4	35.8
Urata et al [66]	p-Ca$_{2.7}$Bi$_{0.3}$Co$_4$O$_9$ n-CaMn$_{0.98}$Mo$_{0.02}$O$_3$	8	Ag paste	897	565	1	170	5 × 5 × 4.5	42.5
Noudem et al [67]	p-Ca$_3$Co$_4$O$_9$ n-Ca$_{0.95}$Sm$_{0.05}$MnO$_3$	2	Ag paste	990	630		31.5	4 × 4 × 10	49.2
Funahashi et al [68]	p-Ca$_{2.7}$Bi$_{0.3}$Co$_4$O$_9$ n-La$_{0.9}$Bi$_{0.1}$NiO$_3$	1	Ag paste	1073	500	0.1	94	3.7 × 4–4.5	310
Lim et al [70]	p-Ca$_3$Co$_4$O$_9$ n-Ca$_{2.9}$Nd$_{0.1}$MnO$_3$	1	Ag paste	1175	727		95	8.5 × 6.0	93.2
Han et al [69]	p-Ca$_3$Co$_{3.8}$Ag$_{0.2}$O$_9$ n-Ca$_{0.98}$Sm$_{0.02}$MnO$_3$	2	Ag paste +5 wt% CaMnO$_3$	873	523	0.3	36.8	3 × 6 × 6	49.1
Funahashi and Mikami [71]	p-Ca$_{2.7}$Bi$_{0.3}$Co$_4$O$_9$ n-La$_{0.9}$Bi$_{0.1}$NiO$_3$	140	Ag paste	1072	551	4.5	150	1.3 × 1.3 × 5	31.7
Choi et al [72]	p-Ca$_3$Co$_4$O$_9$ n-(ZnO)$_7$In$_2$O$_3$	44	Ag paste	1100	658	1.8	423	15 × 15	2.1
Mele et al [73]	p-Ca$_3$Co$_4$O$_9$ n-Zn$_{0.98}$Al$_{0.02}$O	6	Ag	773	260	0.3	3.7	5 × 5 × 15	< 0.1
This work	p-Ca$_3$Co$_4$O$_9$ n-Zn$_{0.98}$Al$_{0.02}$O	8	Ag paste and foil hot-press	906	496	0.7	65.3	3 × 3 × 8	45.3

Van, Pryds ANSNN 2013

(Zn, Al)O
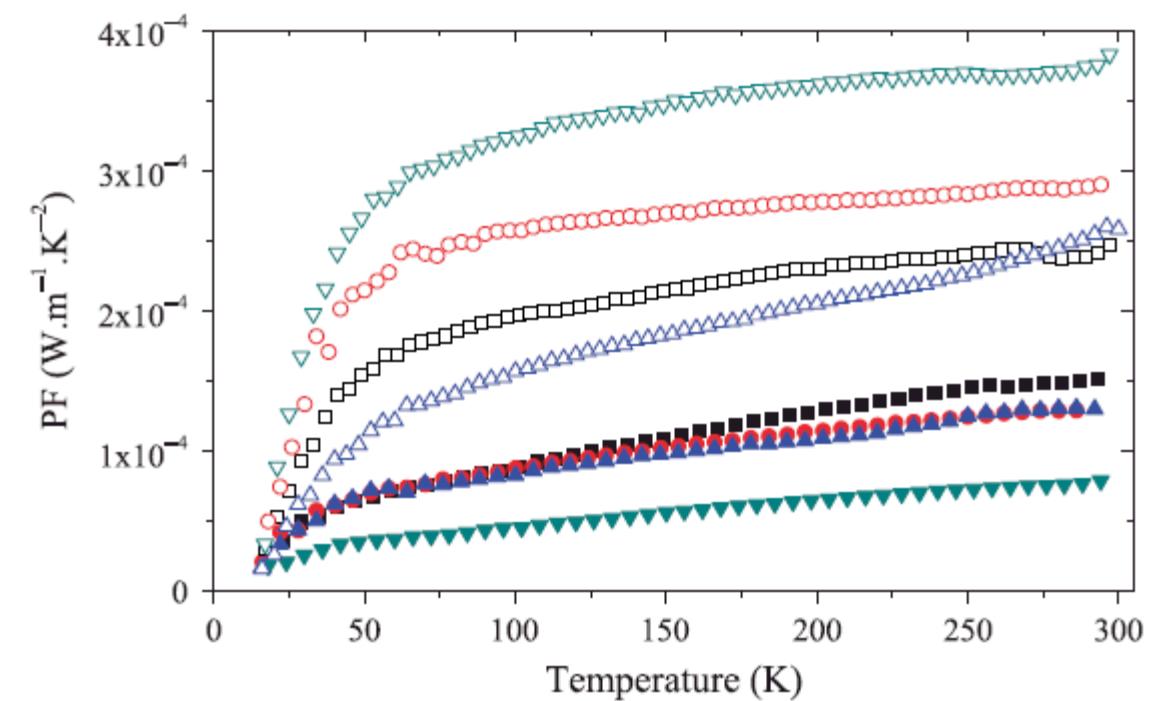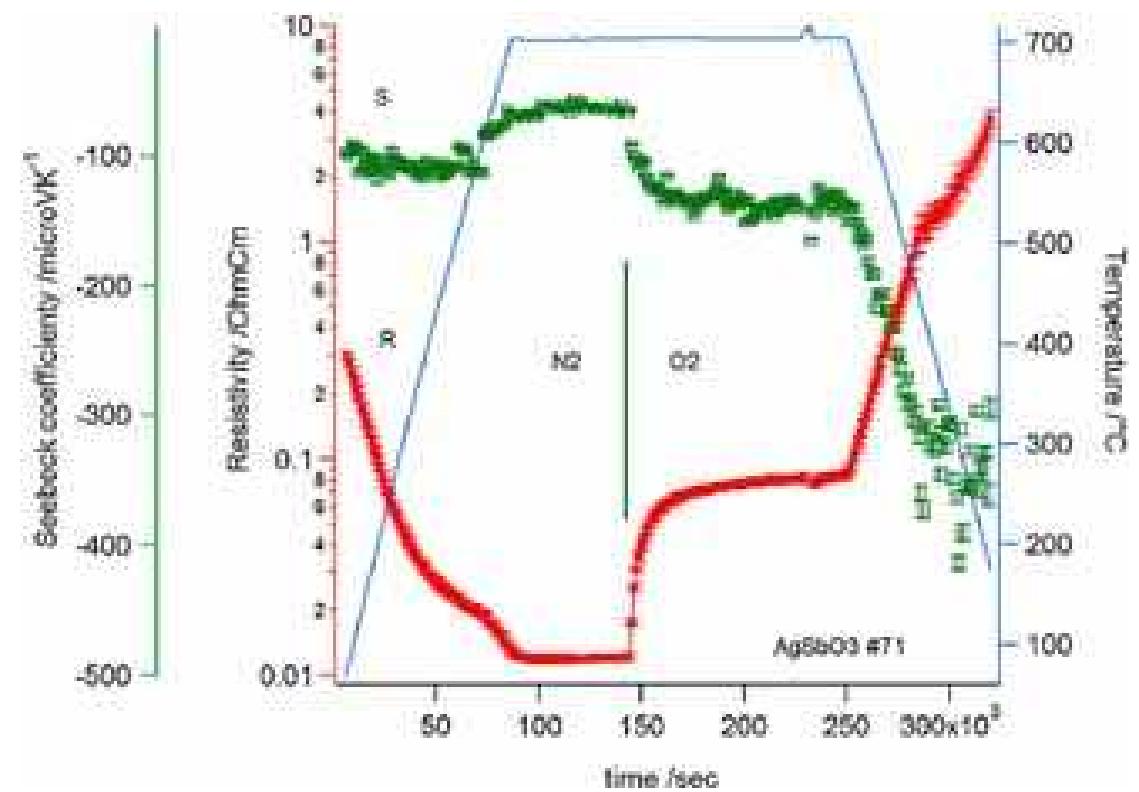
Bérardan, Byl, Dragoe, J. Am. Ceram. Soc. 2010

AgSbO₃

Dragoe, Berardan, Byl PSS-A 2010

(Zn, Al)O
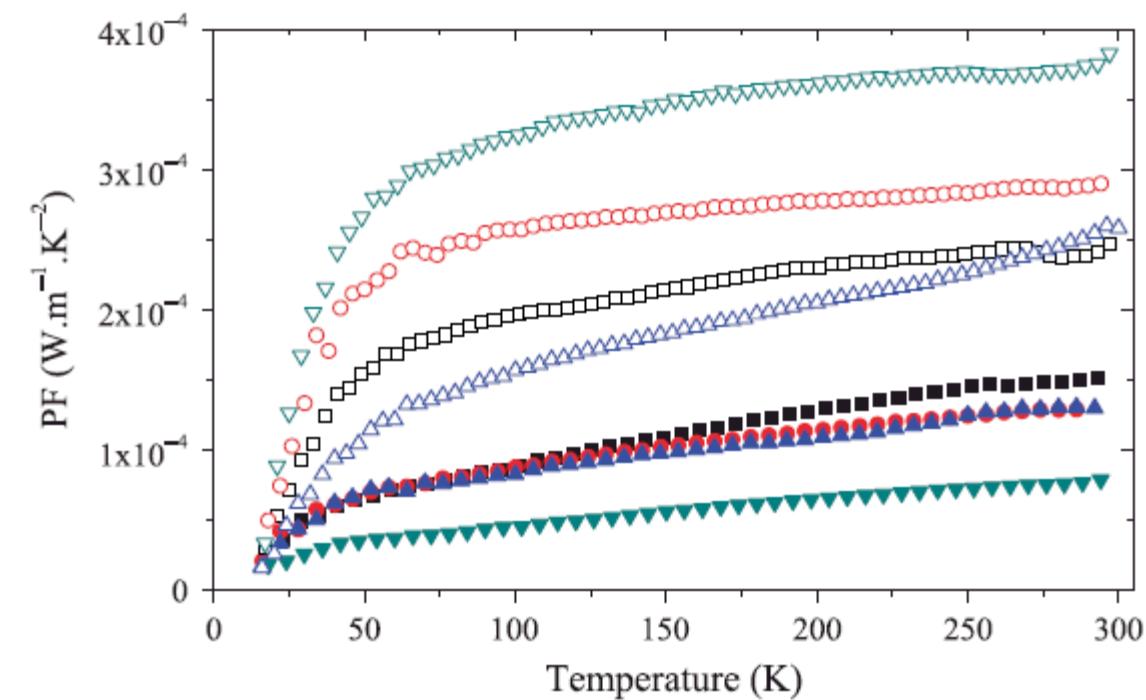
Bérardan, Byl, Dragoe, J. Am. Ceram. Soc. 2010

AgSbO$_3$
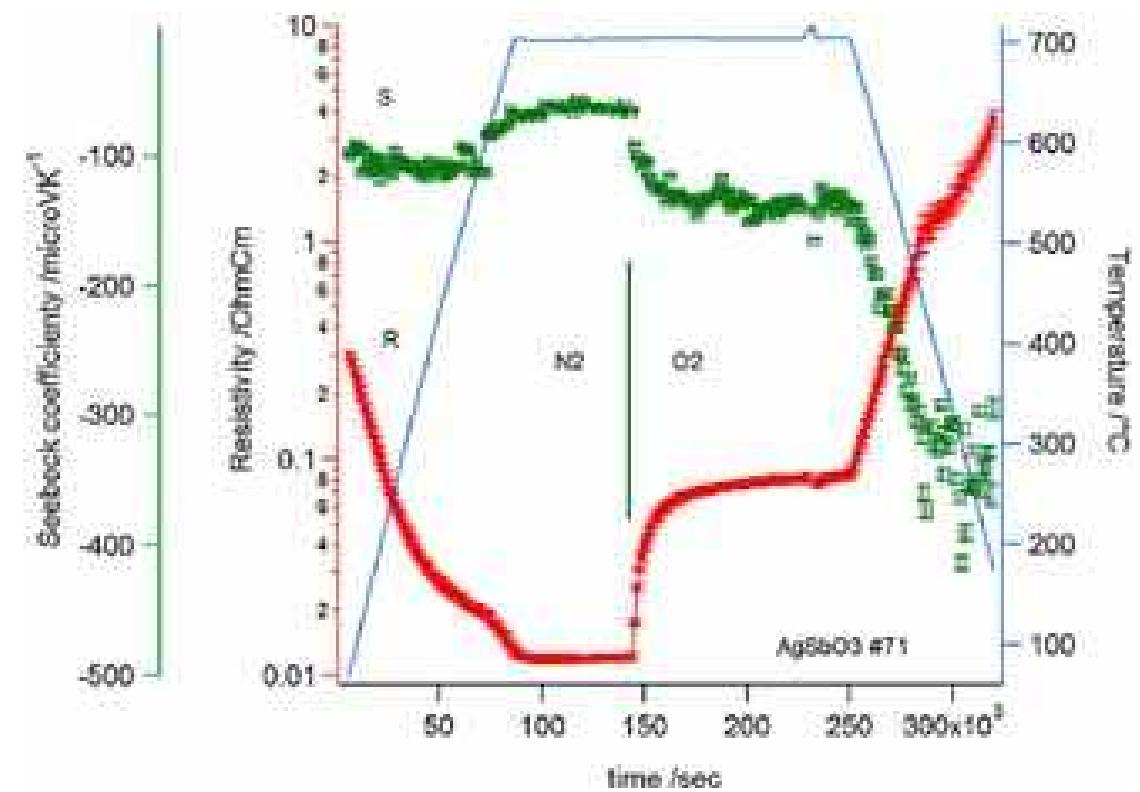
Dragoe, Berardan, Byl PSS-A 2010

Why does this happen, how do you model the stability of oxides in air?

Materials are unstable in different atmospheres due to <u>Defects</u>

Defects are always present in materials

-Lowering of Gibbs free energy through increased entropy

-It is impossible to make a perfect crystal

-for TE, we need dopants, which lead to defects by definition

-polycrystalline materials are usually used for applications

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Relevance for thermoelectrics:

-Defects compensate donor/acceptor doping, changing carrier concentrations
-True for PbTe, Bi_2Te_3, SiGe, oxides, etc…

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Relevance for oxides "in air"

Defect chemistry changes with prevailing solid-gas equilibrium

Problem: systematically understand stability of oxide thermoelectrics

1. In order to study stability, measure properties as a function of oxygen partial pressure at fixed T:
$pO_2 = 10^{-24}$ to 1 atm
Air: $pO_2 \sim 0.2$ atm
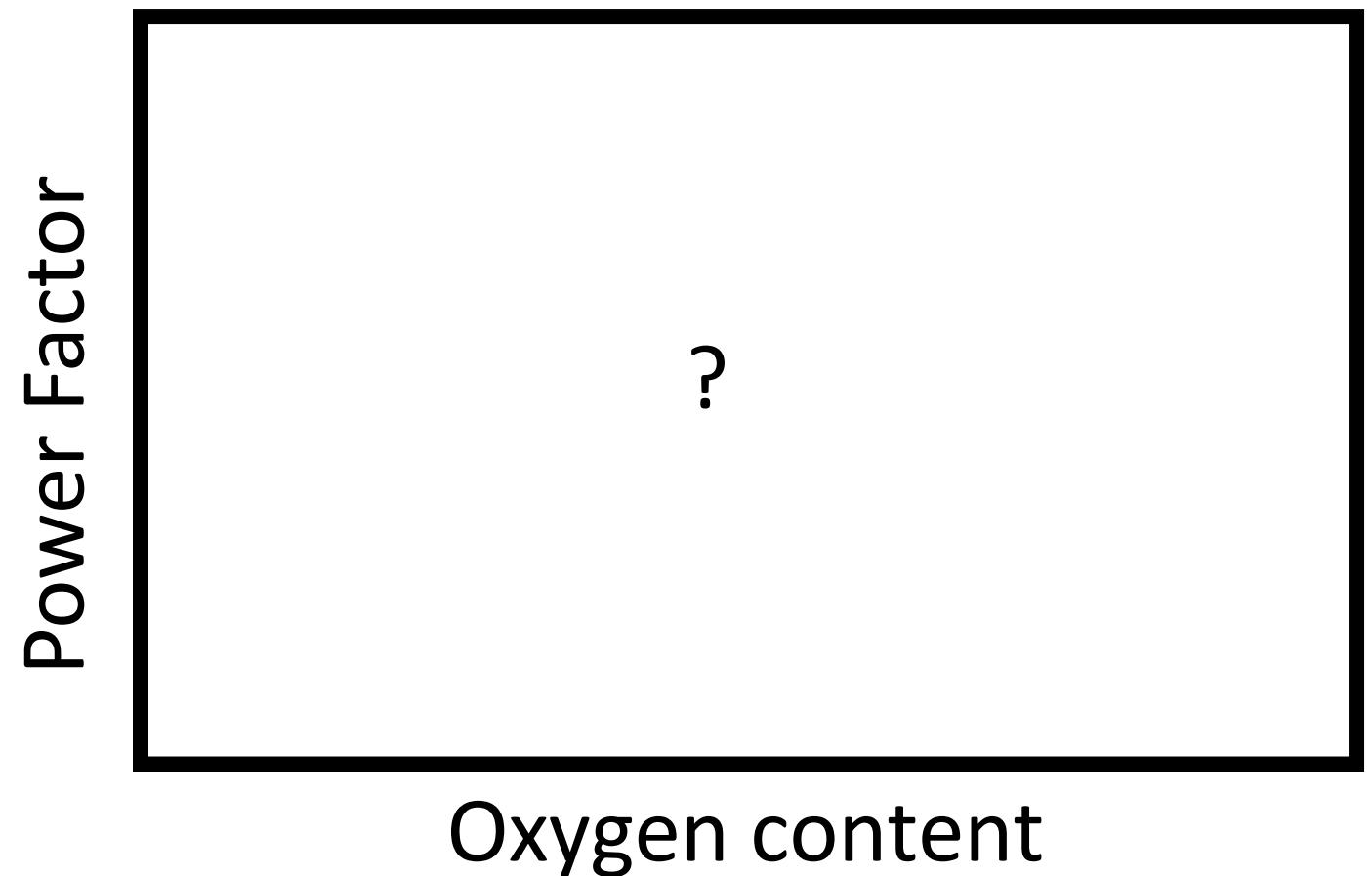
Problem: systematically understand stability of oxide thermoelectrics

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2. Use a thermoelectric oxide with a <u>well-known</u> defect chemistry: Doped $SrTiO_3$ has been studied for more than 40 years and is also a good thermoelectric.
(lots of literature for different temperature ranges!)

Sr(Ti,Nb)O$_3$ is a model system for studying stability

Nb^{5+} replaces Ti^{4+} donating electron to CB

n = N$_D$ = Nb concentration

Extra electron

Conduction Band

Shallow Nb donor level

Valence Band

Nb-4.0 × 10^{21} cm^{-3}

La-7.9 × 10^{20} cm^{-3}

Nb-3.7 × 10^{20} cm^{-3}

Nb-1.6 × 10^{20} cm^{-3}

La-7.0 × 10^{19} cm^{-3}

Dimensionless Figure of Merit, *ZT*

Temperature, *T* (K)

Koumoto *et al*., MRS Bull., **31** (2006)
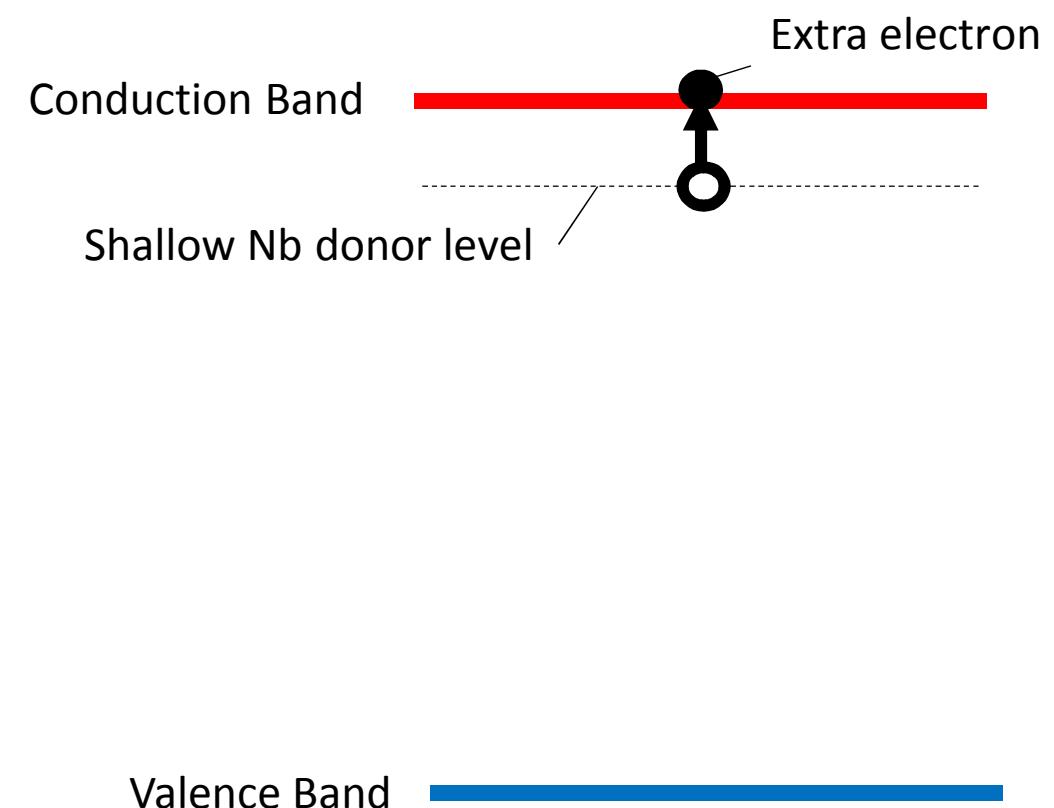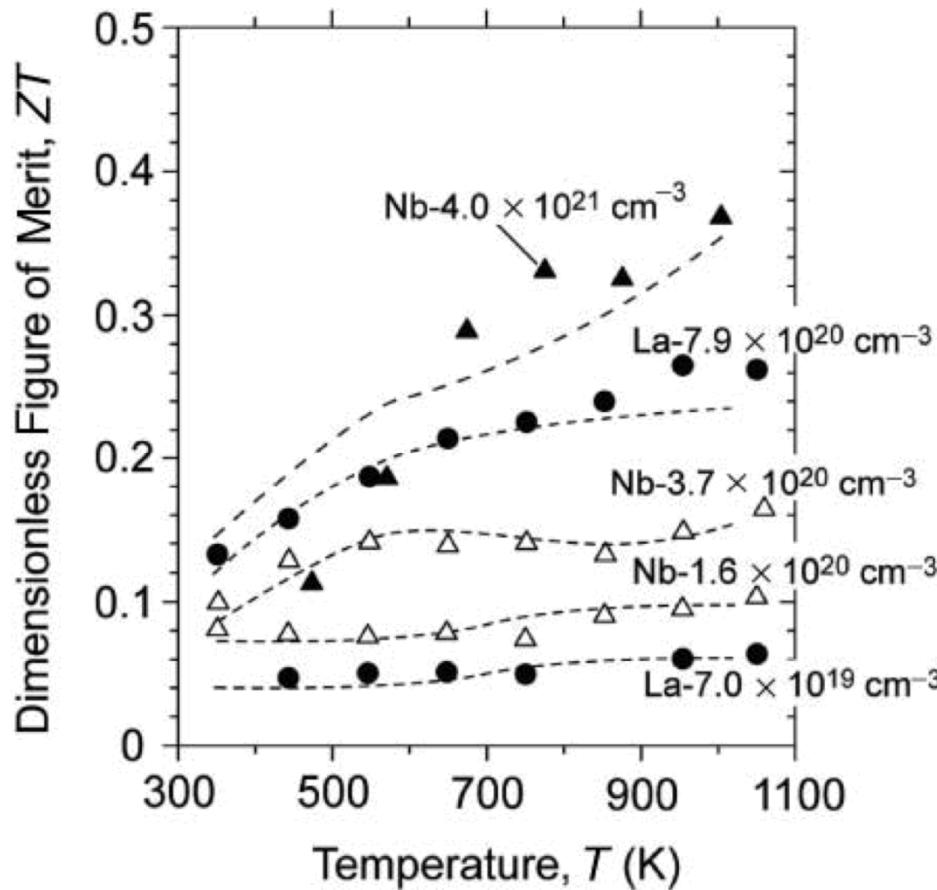
Sr(Ti,Nb)O$_3$

Nb^{5+} replaces Ti^{4+}

Either: More Oxygen or More electrons

In presence of oxygen, excess accommodated by lattice (not interstitial),
introducing <u>acceptor</u> Sr vacancies

Sr ●Ti ○O

$n = 1$ [SrO(SrTiO$_3$)] $n = 2$ [SrO(SrTiO$_3$)$_2$]
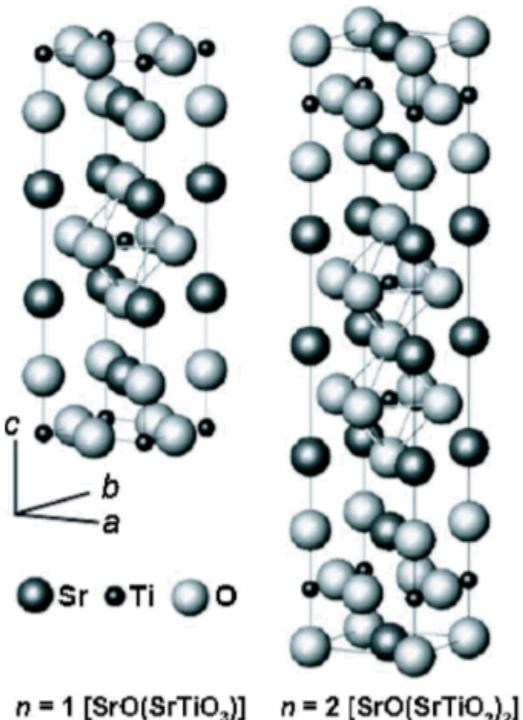
RP mechanism
Lee J. Appl. Phys. 06

Conduction Band

Nb donor

Sr vacancy acceptor

Valence Band
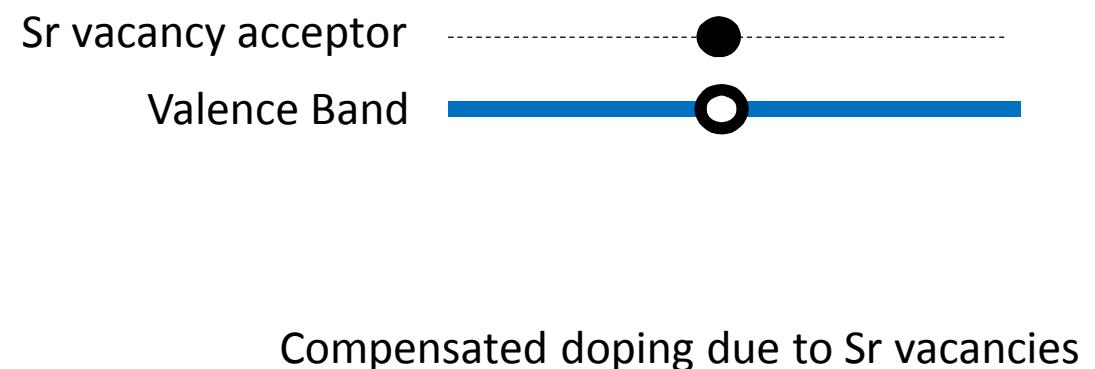
Compensated doping due to Sr vacancies

Sr(Ti,Nb)O$_3$

Nb^{5+} replaces Ti^{4+}

Either: More Oxygen or More electrons

At low oxygen levels, Sr vacancies disappear.

Instead, oxygen vacancies form, which are double donors

Conduction Band

Nb donor

O vacancy donor

Valence Band

Oxygen vacancies add further carriers
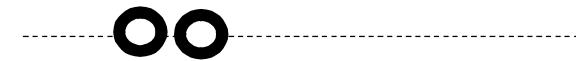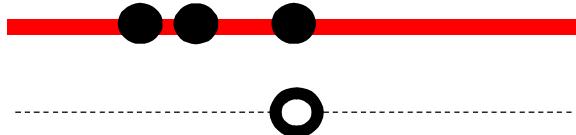
Overview of Defect Chemistry in Donor doped SrTiO$_3$ (Simplified!)

[1] Oxygen Vacancy Formation:

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

Cf. Moos, Hardtl, JACerS 1997

[2] Strontrium Vacancies:

$$Sr_{Sr}^x + O_O^x \rightleftharpoons V_{Sr}'' + V_O^{\cdot\cdot} + SrO_{RP}$$
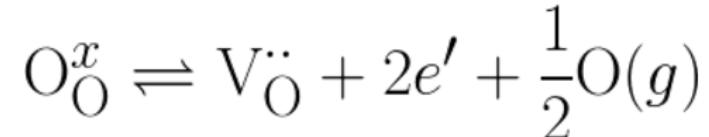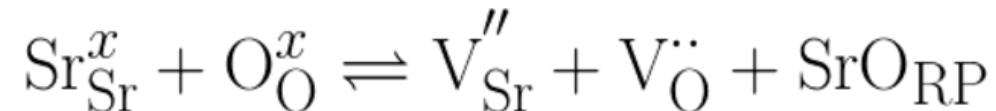
[3] Intentional, extrinsic dopants (Nb)

[4] Electroneutrality (Kroger-Vink notation)

$$n + 2[V_{Sr}''] = 2[V_O^{\cdot\cdot}] + [Nb_{Ti}^{\cdot}] + p$$

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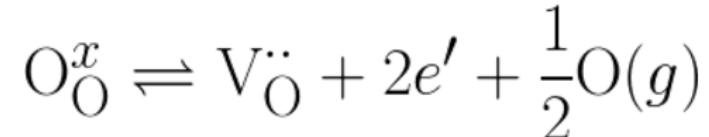
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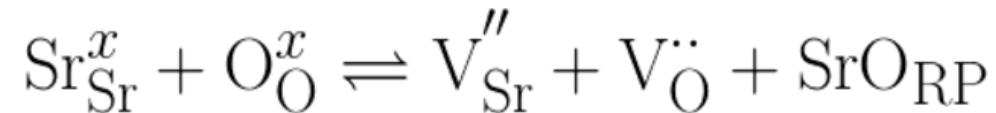
[3] Nb dopants

Key point: these are all coupled and dependent upon prevailing oxygen partial pressure

[4] Electroneutrality (Kroger-Vink notation)

$$n + 2[V_{Sr}''] = 2[V_O^{\cdot\cdot}] + [Nb_{Ti}^{\cdot}] + p$$

$$n + 2[V''_{Sr}] = 2[V_O^{\cdot\cdot}] + [Nb_{Ti}^{\cdot\cdot}] + p$$

(with $2[V''_{Sr}]$ and $[Nb_{Ti}^{\cdot\cdot}]$ crossed out)

$$O_O^x \rightleftharpoons V_O^{\cdot\cdot} + 2e' + \frac{1}{2}O(g)$$
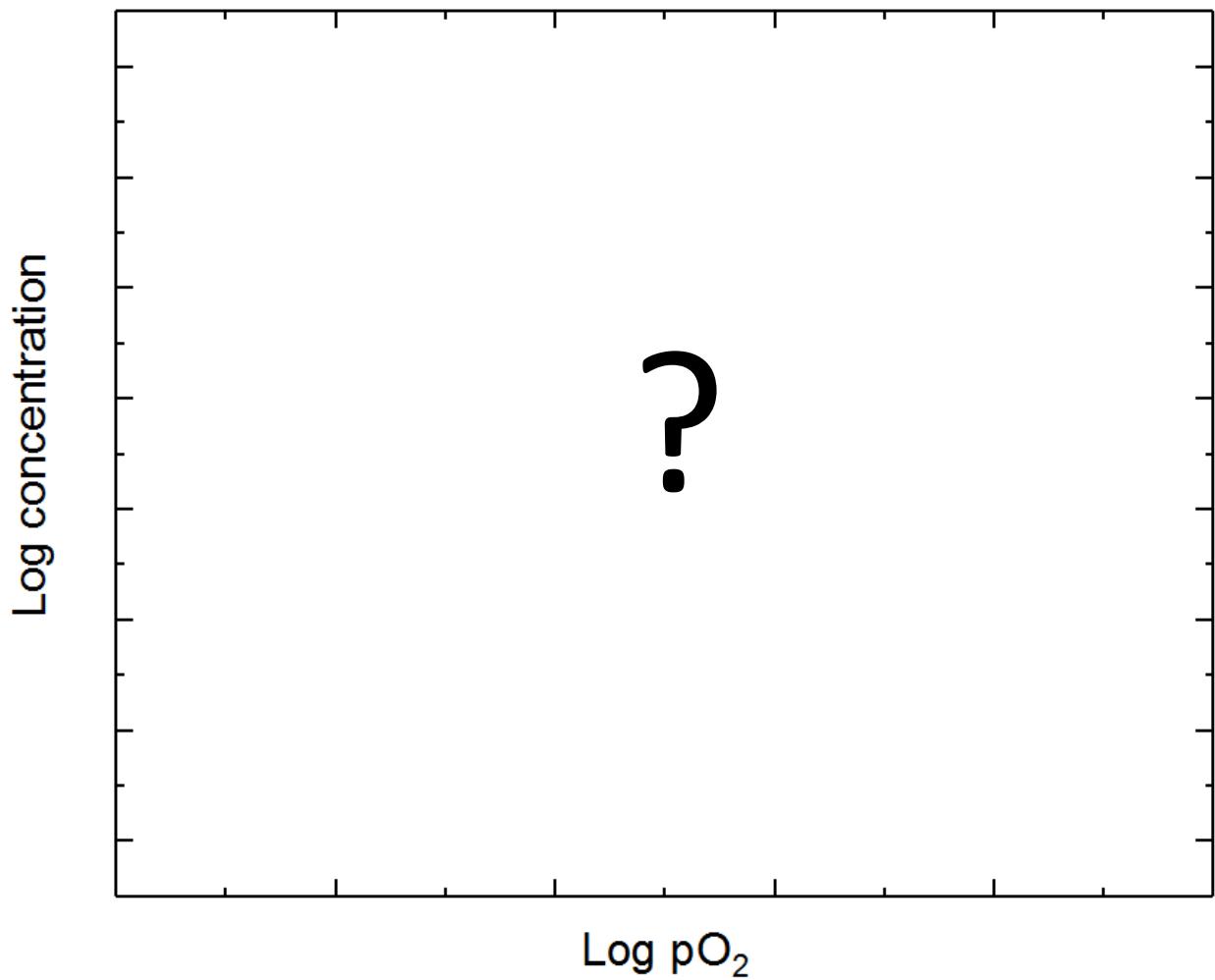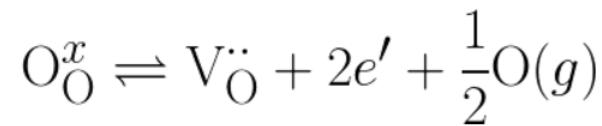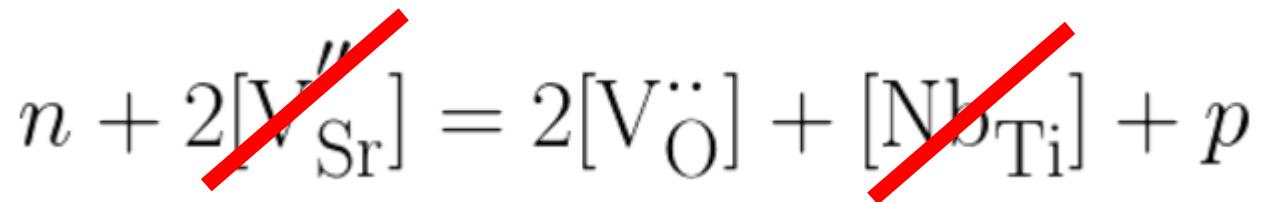
Principle of Mass Action:

$$[V_O^{\cdot\cdot}] \, n^2 \, pO_2^{1/2} = K_1$$

$$[V''_{Sr}][V_O^{\cdot\cdot}] = K_2$$

$$n \sim 2[V_O^{\cdot\cdot}]$$

$$n \sim pO_2^{-1/6}$$
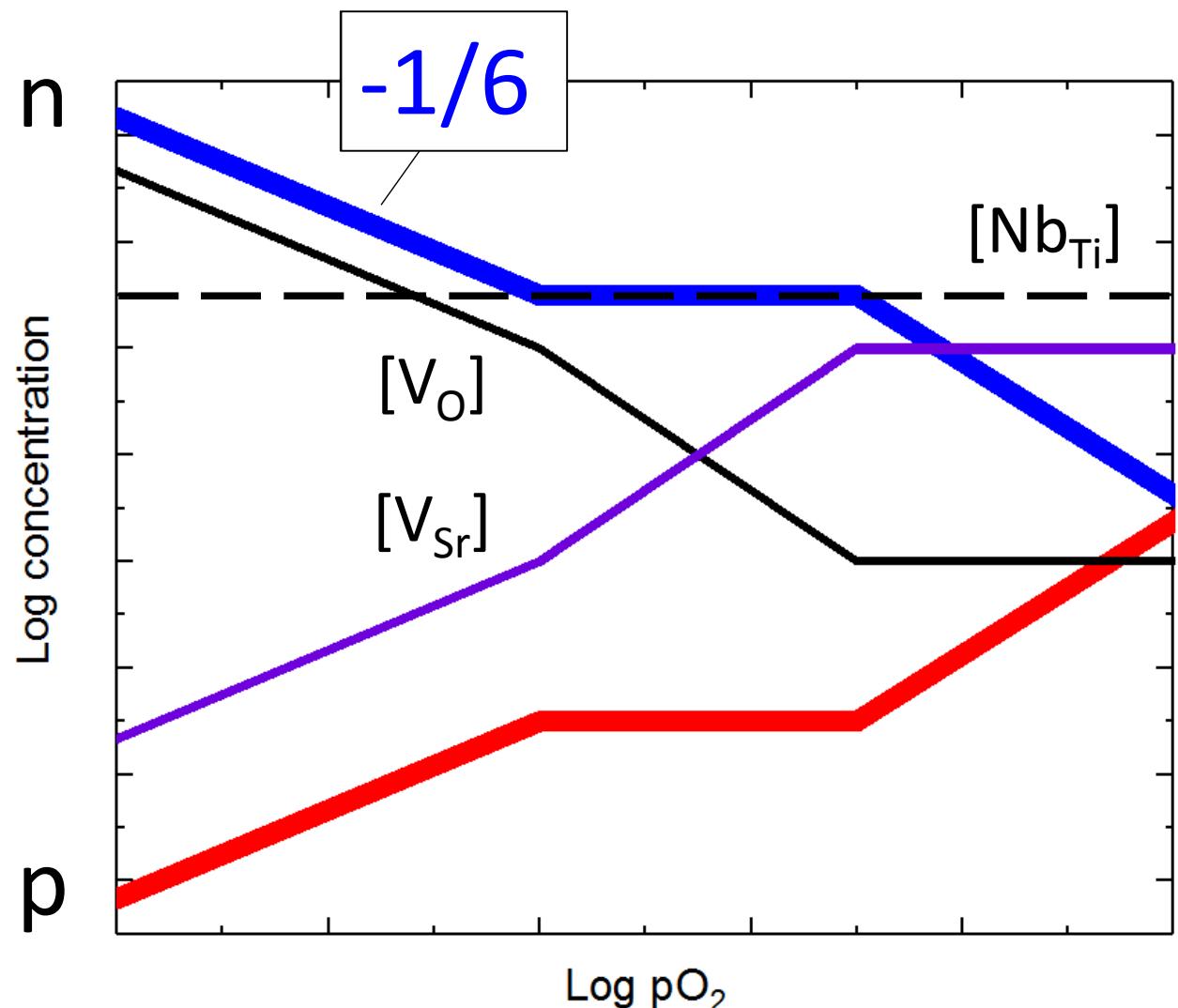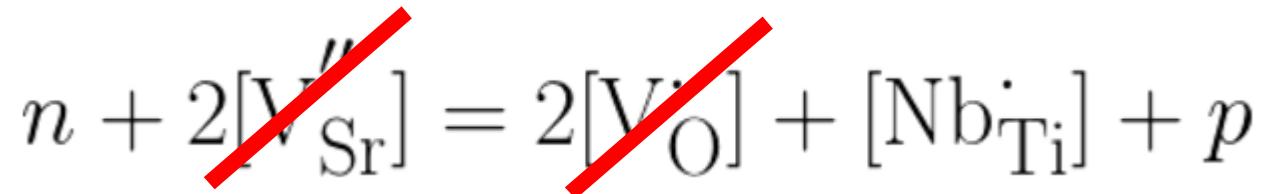
$$n + 2[V''_{Sr}] = 2[V^{\cdot\cdot}_{O}] + [Nb^{\cdot}_{Ti}] + p$$

$$n \sim [Nb^{\cdot}_{Ti}]$$

$$n + 2[V''_{Sr}] = 2[V^{\cdot\cdot}_O] + [Nb^{\cdot}_{Ti}] + p$$
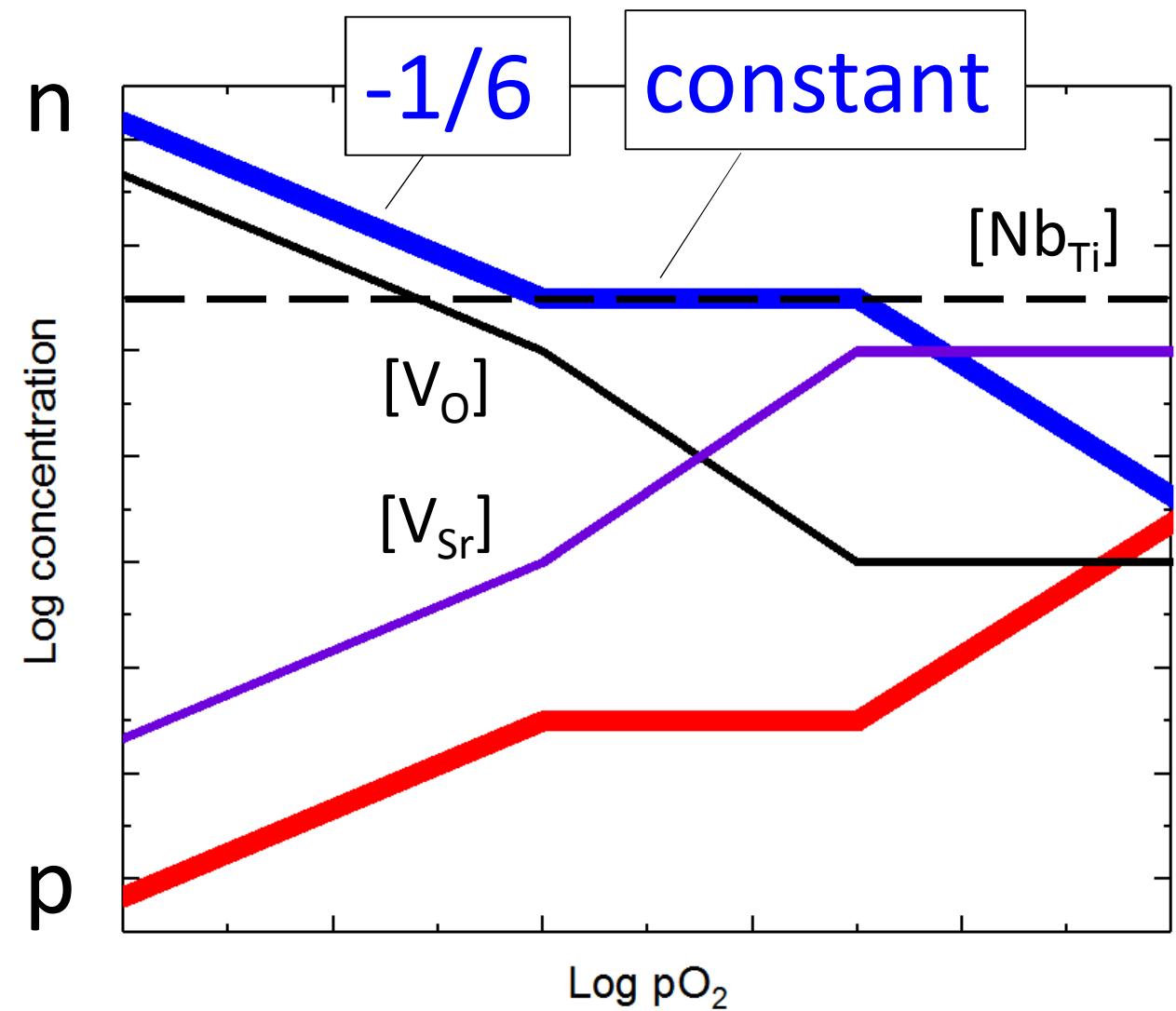
$$Sr^x_{Sr} + O^x_O \rightleftharpoons V''_{Sr} + V^{\cdot\cdot}_O + SrO_{RP}$$
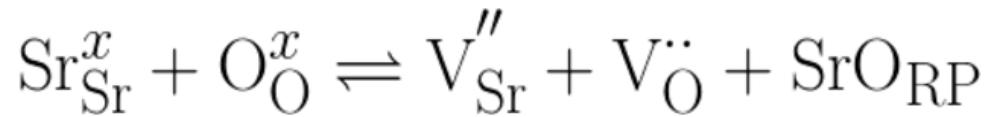
Principle of Mass Action:

$$[V''_{Sr}][V^{\cdot\cdot}_O] = K_2$$

$$[V^{\cdot\cdot}_O]\, n^2\, pO_2^{1/2} = K_1$$

$$2[V_{Sr}''] \sim [Nb^{\cdot}_{Ti}]$$

$$n \sim pO_2^{-1/4}$$

-1/6 constant

n

[Nb_Ti]

[V_O]

[V_Sr]

-1/4

p

Log concentration

Log pO₂
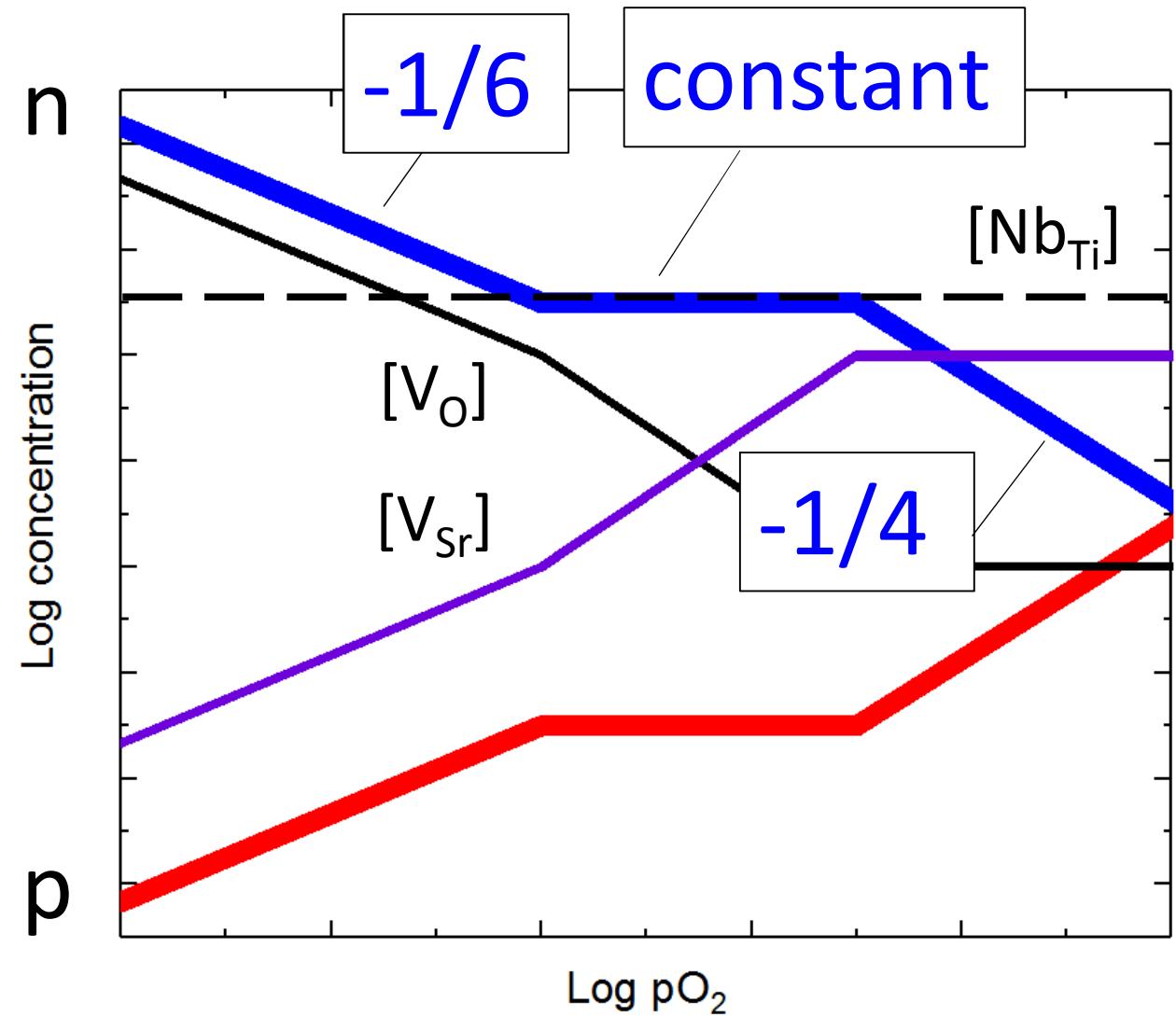
pO$_2$ changes carrier concentration, changing transport properties

Moos, Hardtl JACeRS 97
(La,Sr)TiO$_3$

$$\sigma = ne\mu$$
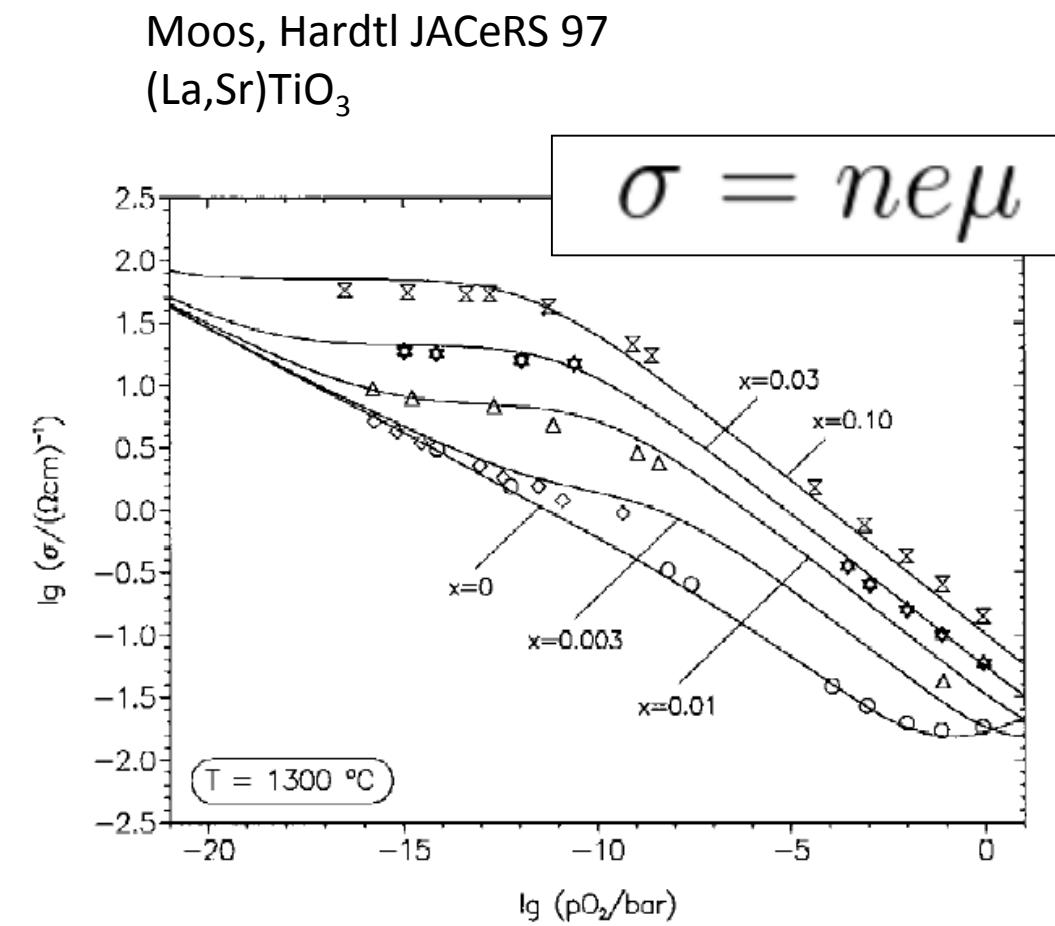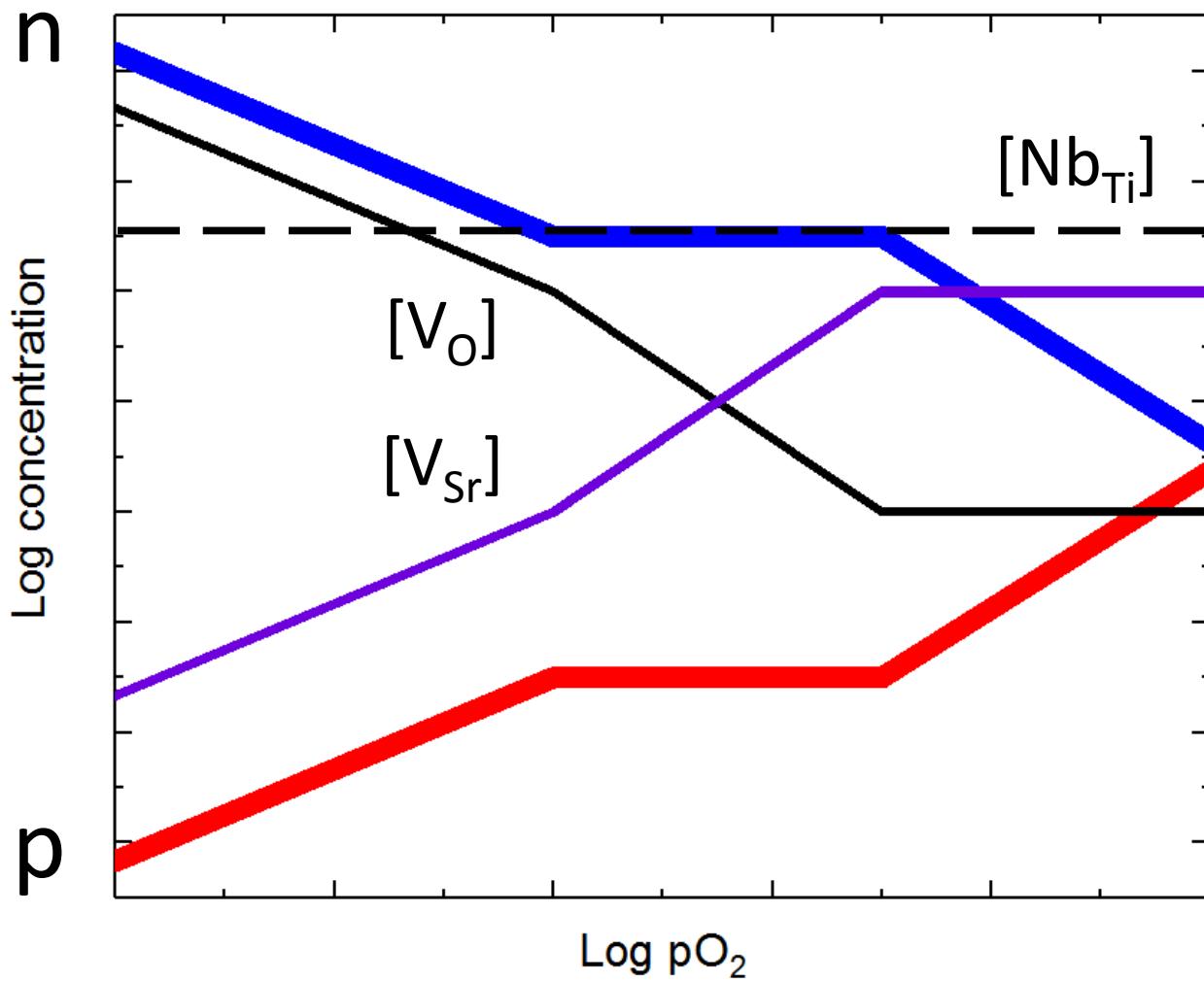
pO$_2$ dependent Conductivity and Seebeck coefficient
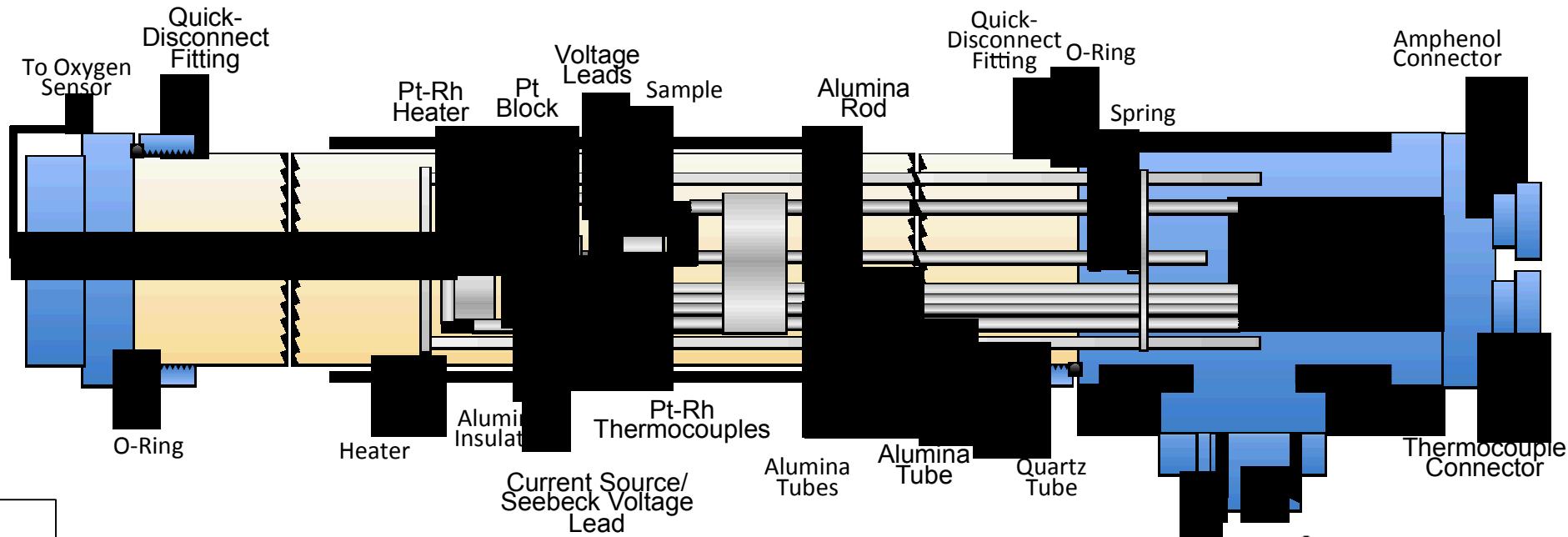
HBS, PAS, JFI
J. Mat Sci. 2015

- All platinum wiring for broad oxygen activity compatibility

- MFC gas control with O$_2$, N$_2$, and 3% H$_2$/N$_2$ providing 1 atm to 10^{-23} atm O$_2$ partial pressure control

- pO$_2$ monitor on instrument exhaust

See also: Byl, Bérardan, Dragoe, Meas. Sci. Tech. 2012
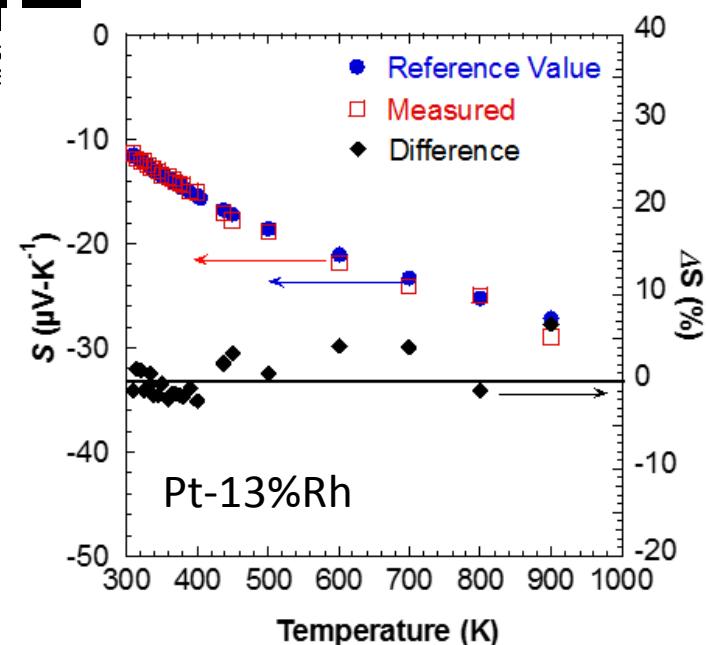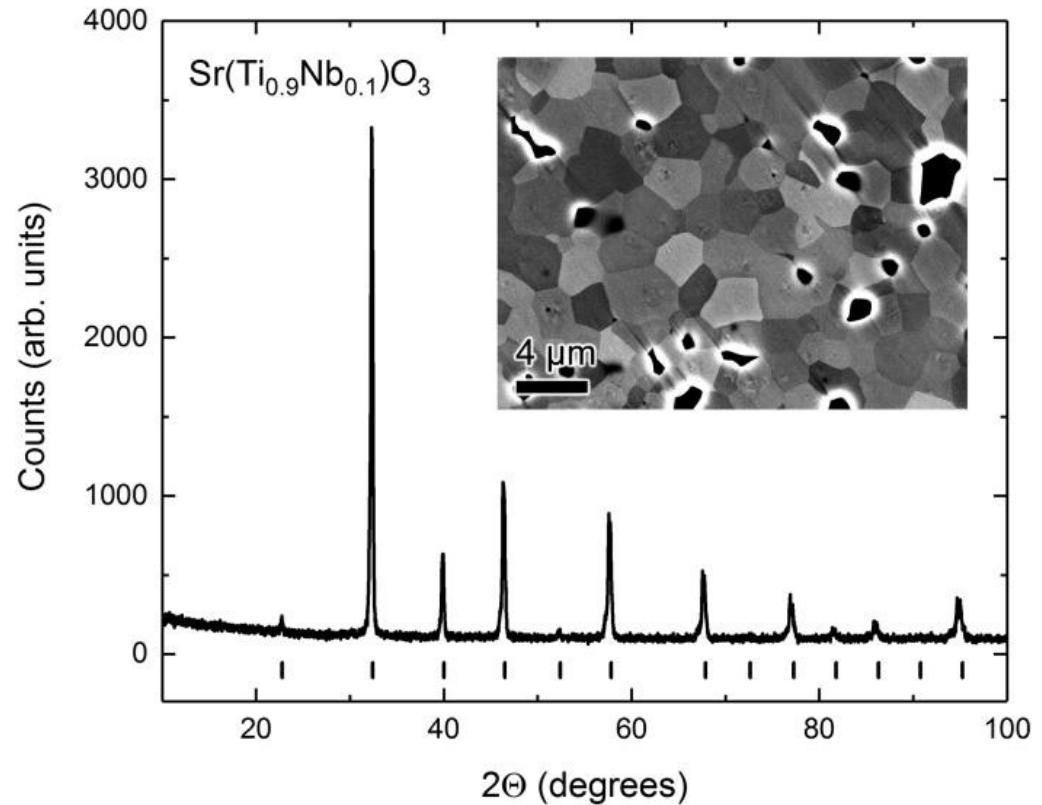
-10% Nb doped $SrTiO_3$ ceramic (prep. In reduced state)
-1% Nb doped $SrTiO_3$ single crystal (prep. In reduced state)
-consistent with previous literature
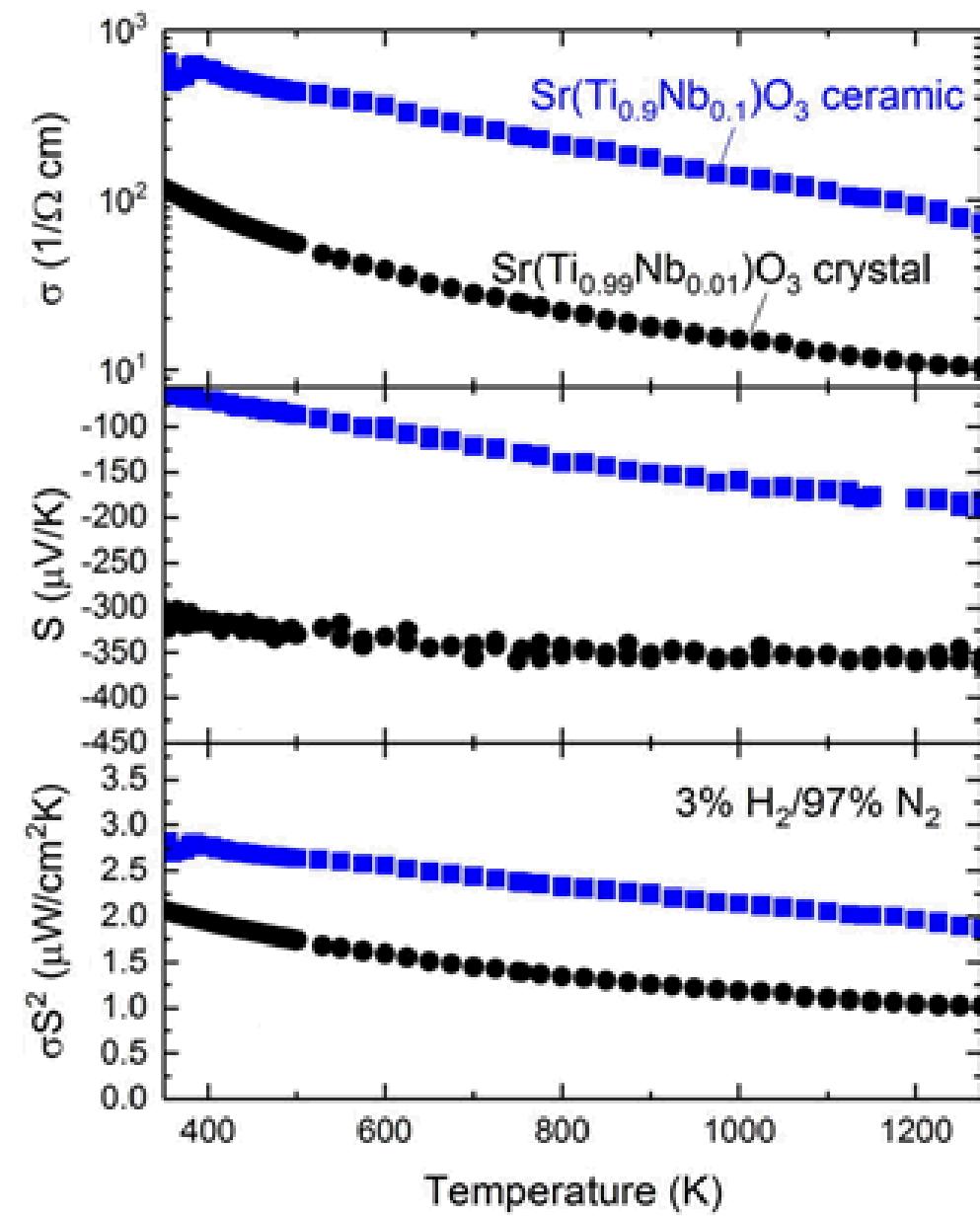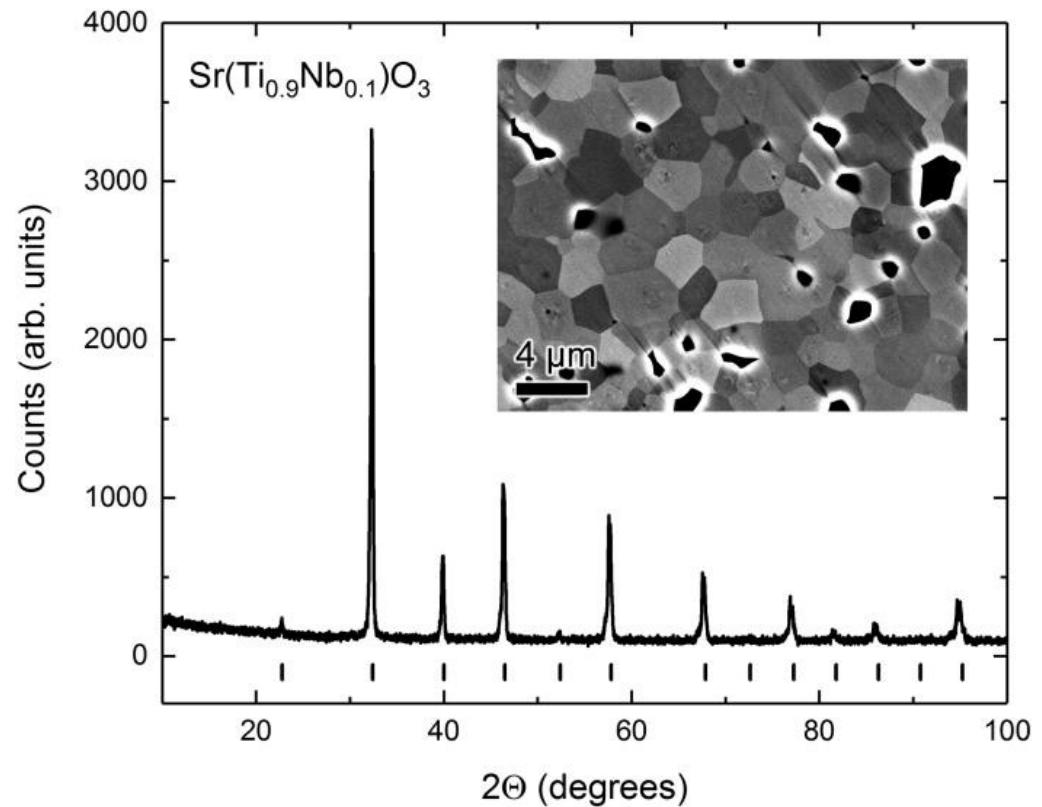
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Oxygen partial pressure?
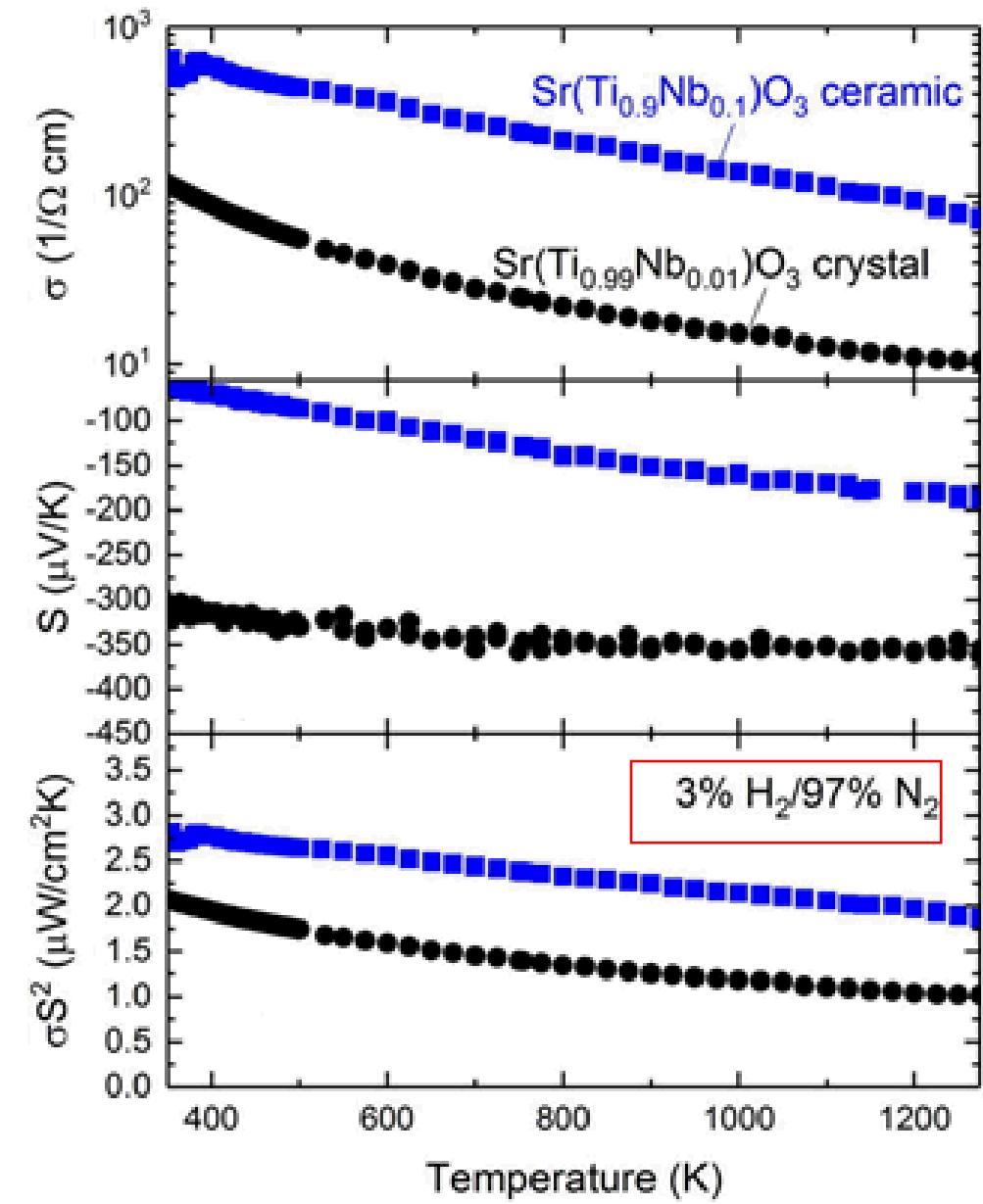
Oxygen partial pressure controlled by gas equilibrium:
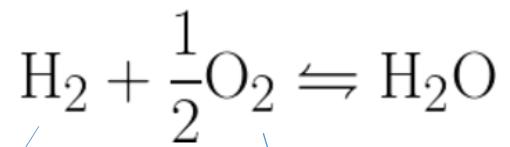
$$H_2 + \frac{1}{2}O_2 \rightleftharpoons H_2O$$

From forming gas mixture

Residual oxygen depending on source

Mass action:

$$\frac{pH_2O}{pH_2 \, pO_2^{1/2}} = K(T)$$

Ceramic
10% Nb doped SrTiO$_3$

Limit of oxygen sensor

Simulation based on known K(T)

3% H$_2$/97% N$_2$

Oxygen partial pressure controlled by gas equilibrium:

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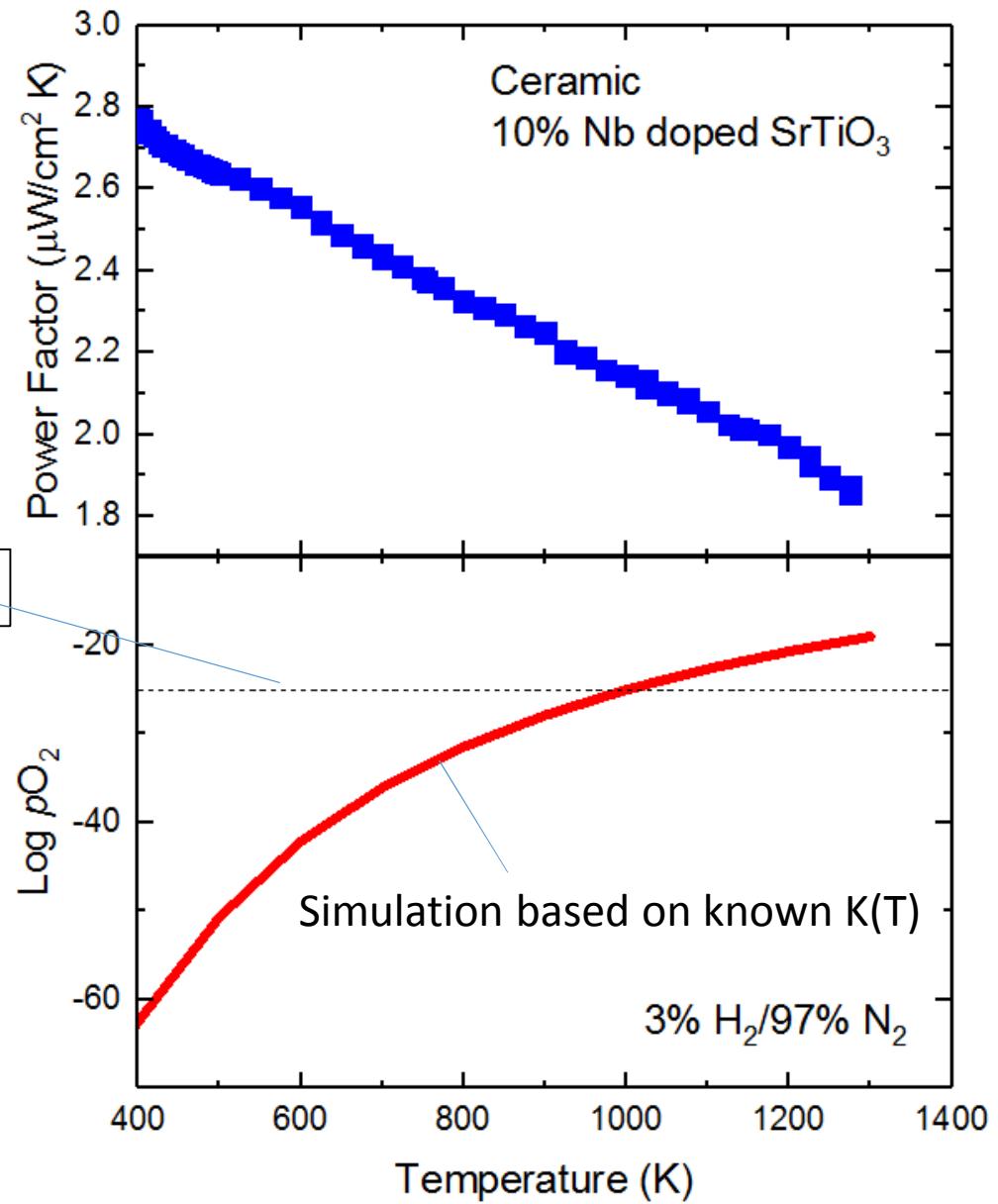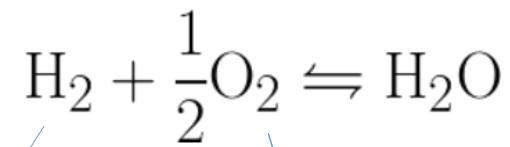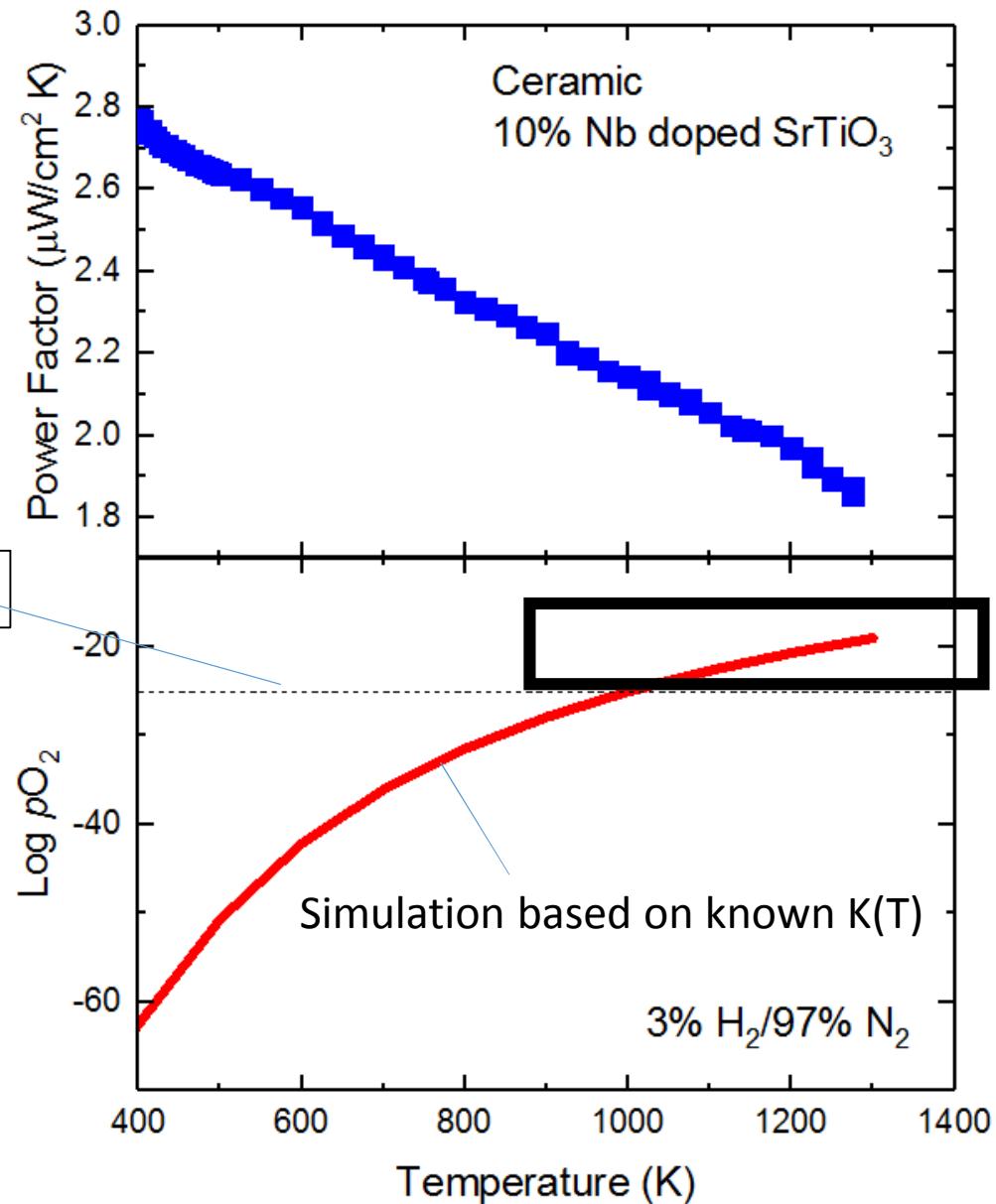
T>1000 K, non-negligible changes in oxygen content v. Temperature
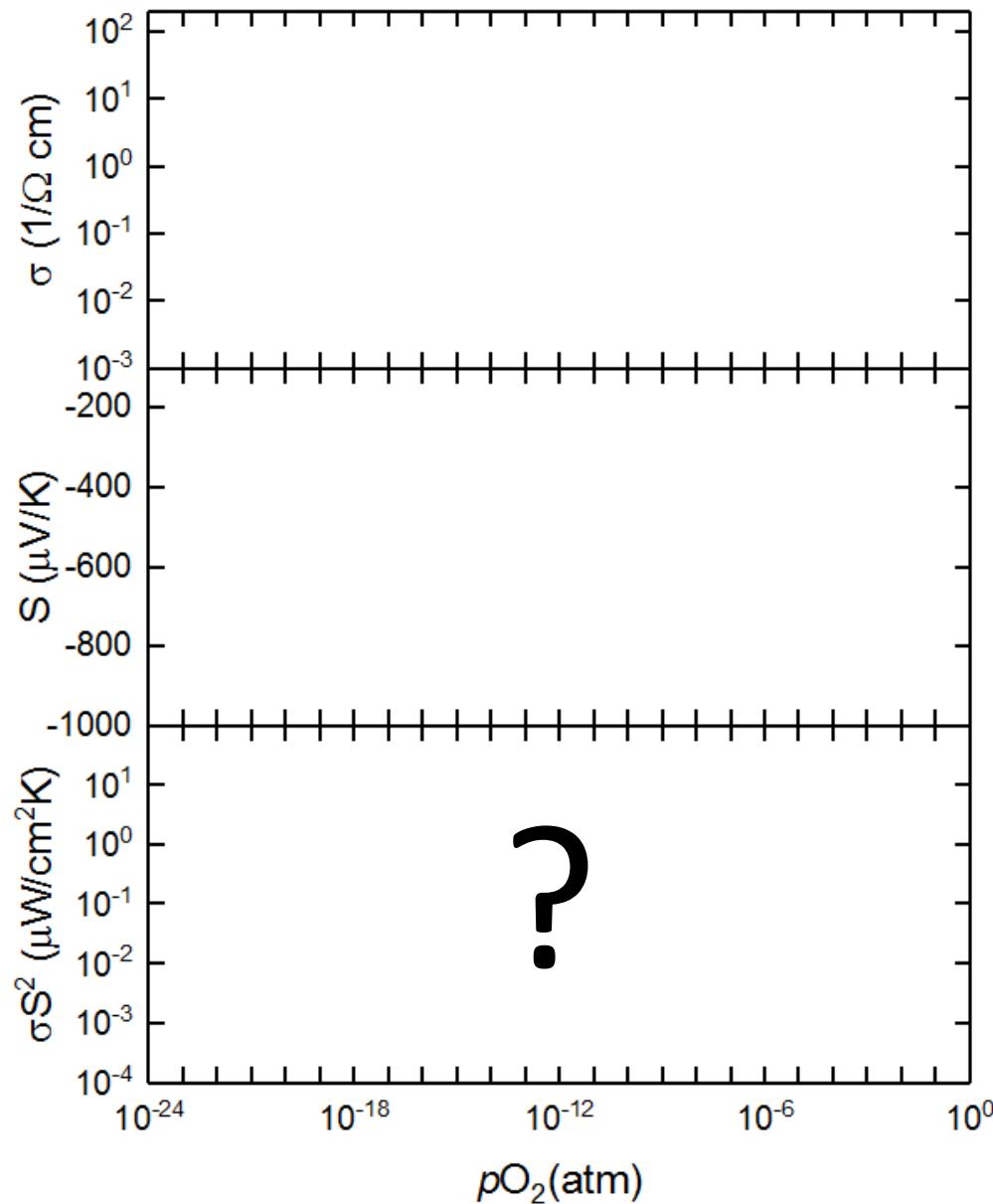
# Isothermal measurements vs. pO$_2$

T = 1173 K

Isothermal measurements vs. pO$_2$
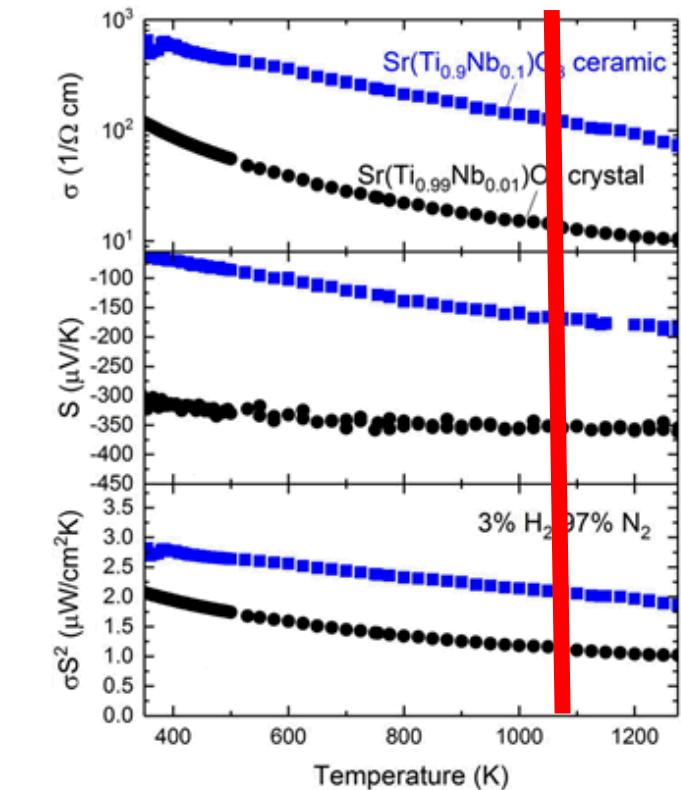
Ceramic 10% Nb-SrTiO$_3$

T = 1173 K

Isothermal measurements vs. pO$_2$

Ceramic 10% Nb-SrTiO$_3$

1 data point = 1 day!

3% H$_2$ 97% N$_2$

T = 1173 K

Isothermal measurements vs. pO$_2$

Ceramic 10% Nb-SrTiO$_3$

Reversible pO2 dependence

T = 1173 K

Isothermal measurements vs. pO$_2$

Ceramic 10% Nb-SrTiO$_3$

Sr(Ti$_{0.9}$Nb$_{0.1}$)O$_3$ ceramic

Sr(Ti$_{0.99}$Nb$_{0.01}$)O$_3$ crystal

3% H$_2$ 97% N$_2$

4 orders of magnitude decrease

T = 1173 K

Isothermal measurements vs. pO$_2$


Xtal 1% Nb-SrTiO$_3$

Ceramic 10% Nb-SrTiO$_3$

T = 1173 K

Isothermal measurements vs. pO_2


Xtal 1% Nb-SrTiO$_3$

Ceramic 10% Nb-SrTiO$_3$

Ceramic is strongly pO_2 dependent
Xtal is not

T = 1173 K

Isothermal measurements vs. pO_2
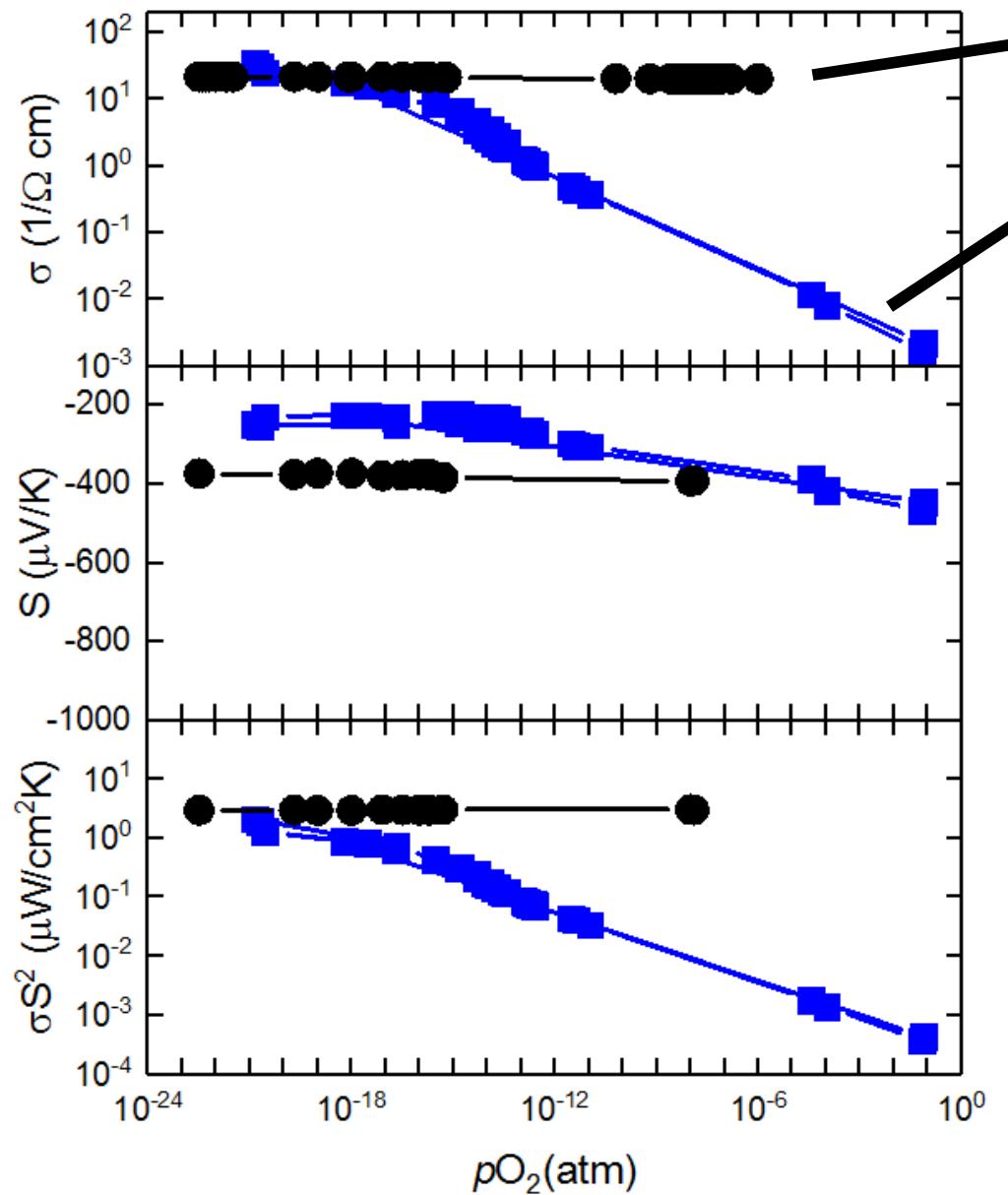
Xtal 1% Nb-SrTiO$_3$

Ceramic 10% Nb-SrTiO$_3$

Ceramic is strongly pO_2 dependent
Xtal is not

What is expected from defect chemistry?

T = 1173 K

Defect Chemistry of Donor-Doped and Undoped Strontium Titanate Ceramics between 1000° and 1400°C

Ralf Moos[†] and Karl Heinz Härdtl[*]

Universität Karlsruhe, Institut für Werkstoffe der Elektrotechnik, D-76128 Karlsruhe, Germany

Defect model, Rate constants summarized in
Moos, Hardtl JACeRS 1997

Table I. System of Equations, Its Set of Constants, and Origin of Constants

Equations (mass-action laws)	Constants used for calculations	Remarks
$[V_{\ddot{O}}]n^2 P_{O_2}^{1/2} = K_{Red}(T) = K_{Red}^{\circ} \exp\left(-\dfrac{\Delta H_{Red}}{kT}\right)$	$K_{red}^{\circ} = 5 \times 10^{71}\ cm^{-9} \cdot bar^{1/2}$ $\Delta H_{red} = 6.1\ eV$	Determined in this study from conductivity data on undoped single crystals and ceramics
$\dfrac{[V_{\ddot{O}}]n}{[V_{\dot{O}}]} = K_{V_{O1\to2}} = K_{V_{O1\to2}}^{\circ} \exp\left(-\dfrac{E_{V_{O1\to2}}}{kT}\right)$	$K_{V_{O1\to2}}^{\circ} = N_C(T)$ $E_{V_{O1\to2}} = 0.3\ meV$	Minor important parameter; determined in a related paper.[38] Parameter becomes important at temperatures <600°C
$\dfrac{[V_{\dot{O}}]n}{[V_{O}^x]} = K_{V_{Ox\to1}} = K_{V_{Ox\to1}}^{\circ} \exp\left(-\dfrac{E_{V_{Ox\to1}}}{kT}\right)$	$K_{V_{Ox\to1}}^{\circ} = N_C(T)$ $E_{V_{Ox\to1}} = 3\ eV$	Minor important parameter; estimated in a related paper.[38] Parameter may become important at temperatures <4.2 K
$np = K_i(T) = N_C(T)N_V(T) \exp\left(-\dfrac{E_g(0\ K) - \beta_g T}{kT}\right)$	$N_C(T) = 4.1 \times 10^{16}\ cm^{-3}(T/K)^{1.5}$ $N_V(T) = 3.5 \times 10^{16}\ cm^{-3}(T/K)^{1.5}$ $E_g(0\ K) = 3.17\ eV$ $\beta_g = 5.66 \times 10^{-4}\ eV/K$	E_g and β_g have been determined in this study; N_C was determined in a related paper,[11] and N_V was determined from literature[8,9] but augmented by a factor of 1.4 for an even-better fit
$[V_{Sr}''][V_{\ddot{O}}] = K_S(T) = K_S^{\circ} \exp\left(-\dfrac{E_S}{kT}\right)$	$K_S^{\circ} = 3 \times 10^{44}\ cm^{-6}$ $E_S = 2.5\ eV$	Determined in this study from conductivity data on different lanthanum-donor-doped ceramics in oxygen-rich atmospheres
$\dfrac{[V_{Sr}']p}{[V_{Sr}^x]} = K_{V_{Srx\to1}}(T) = K_{V_{Srx\to1}}^{\circ} \exp\left(-\dfrac{E_{V_{Srx\to1}}}{kT}\right)$	$K_{V_{Srx\to1}}^{\circ} = N_V(T)$ $E_{V_{Srx\to1}} = 1.4\ eV$	Minor important parameter, included for completeness. Becomes more important at low temperatures in oxygen-rich atmospheres
$\dfrac{[V_{Sr}'']p}{[V_{Sr}']} = K_{V_{Sr1\to2}}(T) = K_{V_{Sr1\to2}}^{\circ} \exp\left(-\dfrac{E_{V_{Sr1\to2}}}{kT}\right)$	$K_{V_{Sr1\to2}}^{\circ} = N_V(T)$ $E_{V_{Sr1\to2}} = 0.1\ eV$	Minor important parameter, included for completeness. Becomes more important at low temperatures in oxygen-rich atmospheres
$\dfrac{[A']p}{[A^x]} = K_A(T) = K_A^{\circ} \exp\left(-\dfrac{E_A}{kT}\right)$	$K_A^{\circ} = N_V(T)$ $E_A = 0.94\ eV$	Minor important parameter, included for completeness. Becomes more important for acceptor-doped samples at high P_{O_2} and low temperature (literature data[47])
$n + 2[V_{Sr}''] + [V_{Sr}'] + [A'] = p + 2[V_{\ddot{O}}] + [V_{\dot{O}}] + [D^{\cdot}]$		The complete electroneutrality condition links all charged defects

$$[V_O^{\cdot\cdot}]\, n^2\, pO_2^{1/2} = K_1$$

$$[V_{Sr}^{''}][V_O^{\cdot\cdot}] = K_2$$

$$np = N_C N_V e^{-\frac{E_g(T)}{kT}}$$

$$n + 2[V_{Sr}^{''}] = 2[V_O^{\cdot\cdot}] + [Nb_{Ti}^{\cdot}] + p$$

1. Solve for n v. pO$_2$

T = 1173 K

$$n + 2[V''_{Sr}] = 2[V^{\cdot\cdot}_O] + [Nb^{\cdot}_{Ti}] + p$$

1. Solve for n v. pO$_2$

2. Find σ, S for given n

$$\sigma = en\mu_N + ep\mu_P$$

$$S = \frac{k}{e}\left[\frac{\sigma_P}{\sigma}(\ln\frac{N_V}{p} + A_V) - \frac{\sigma_N}{\sigma}(\ln\frac{N_C}{n} + A_C)\right]$$

The various transport parameters, such as μ, A$_V$, A$_C$, were previously reported. Cf. Moos, Hardtl
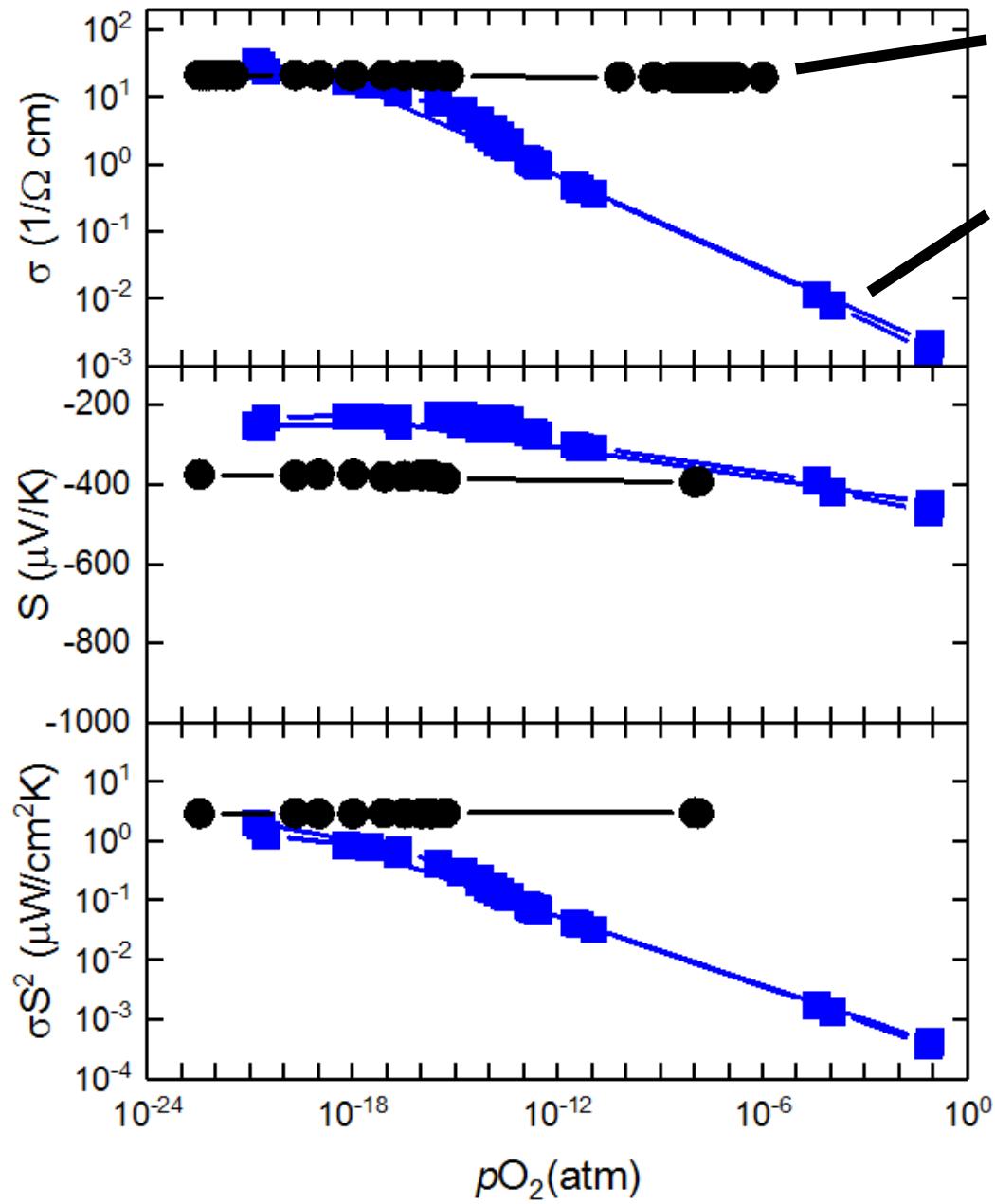
Xtal 1% Nb-SrTiO$_3$

Ceramic 10% Nb-SrTiO$_3$
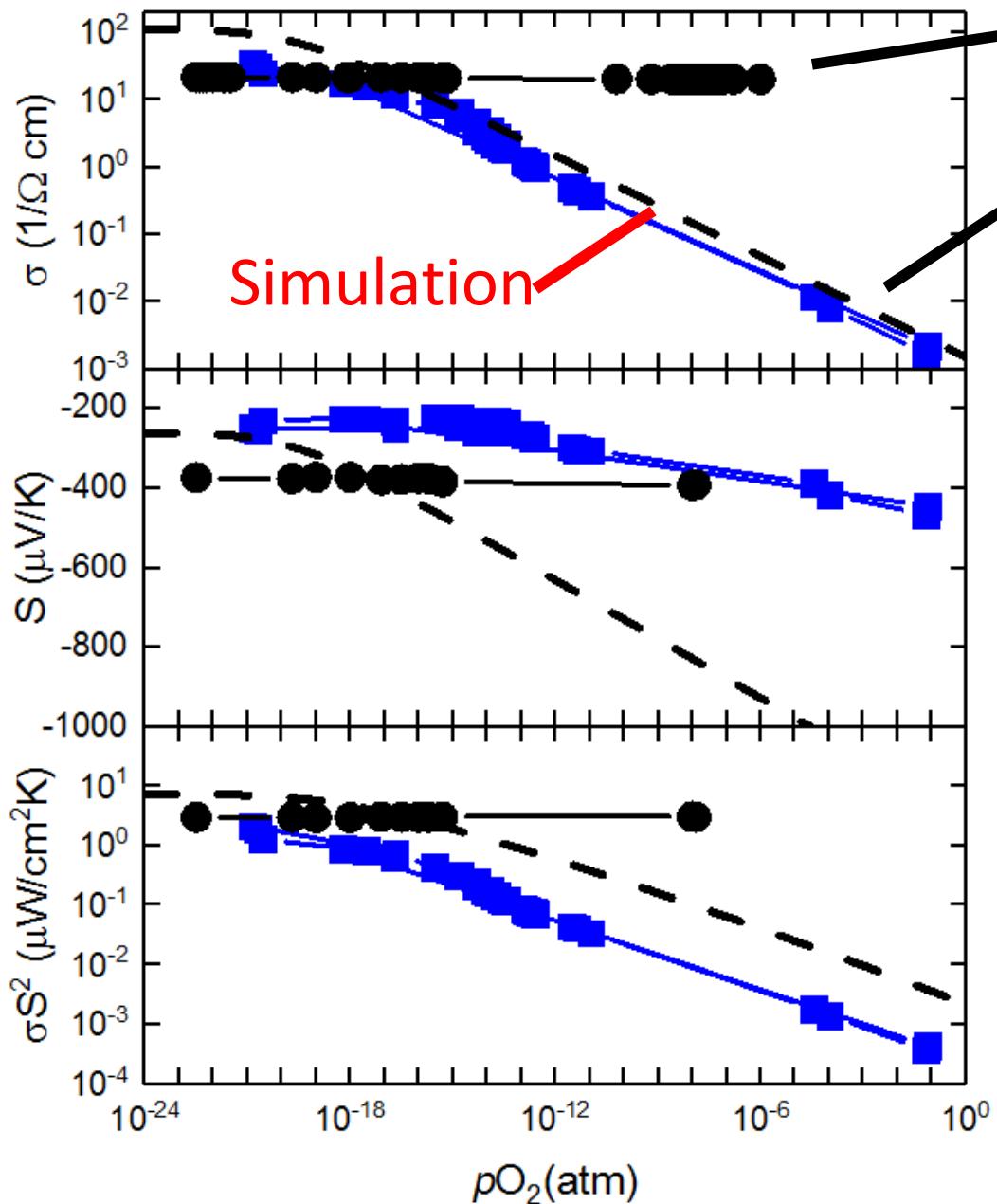
T = 1173 K

Xtal 1% Nb-SrTiO$_3$

Ceramic 10% Nb-SrTiO$_3$

Simulation

$$n + 2[\mathrm{V''_{Sr}}] = 2[\mathrm{V^{\cdot\cdot}_O}] + [\mathrm{Nb^{\cdot}_{Ti}}] + p$$

$$\sigma = en\mu_N + ep\mu_P$$

$$S = \frac{k}{e}\left[\frac{\sigma_P}{\sigma}\left(\ln\frac{N_V}{p} + A_V\right) - \frac{\sigma_N}{\sigma}\left(\ln\frac{N_C}{n} + A_C\right)\right]$$

No curve fitting, constants from Moos, Hardtl for SrTiO$_3$

T = 1173 K
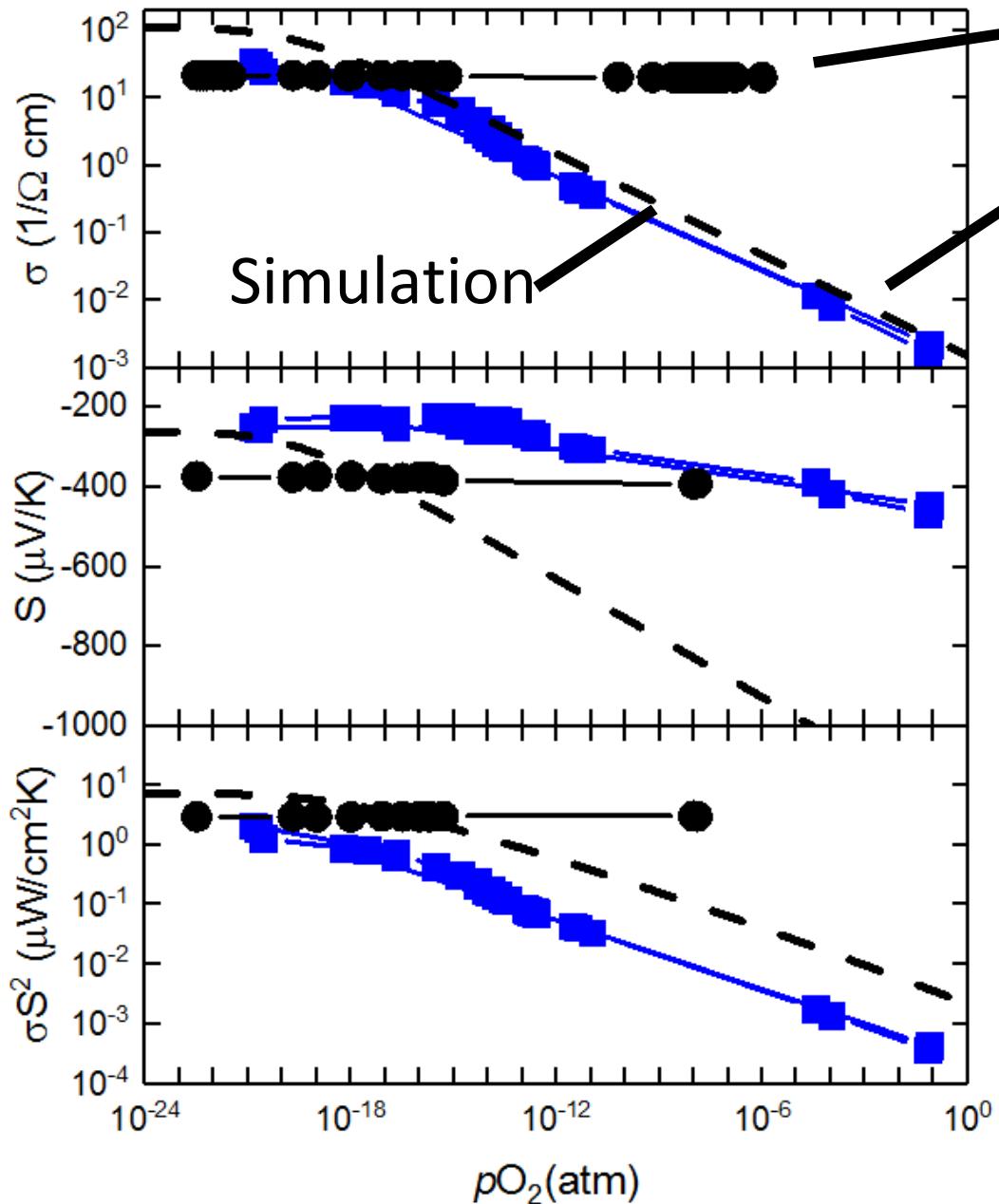
Xtal 1% Nb-SrTiO$_3$

Ceramic 10% Nb-SrTiO$_3$

Simulation

Ceramic is strongly pO$_2$ dependent
Xtal is not

Ceramic similar to Equilibrium Simulation

Difference between Xtal/Ceramic: Kinetics...

T = 1173 K

Xtal 1% Nb-SrTiO$_3$

Ceramic 10% Nb-SrTiO$_3$

Simulation
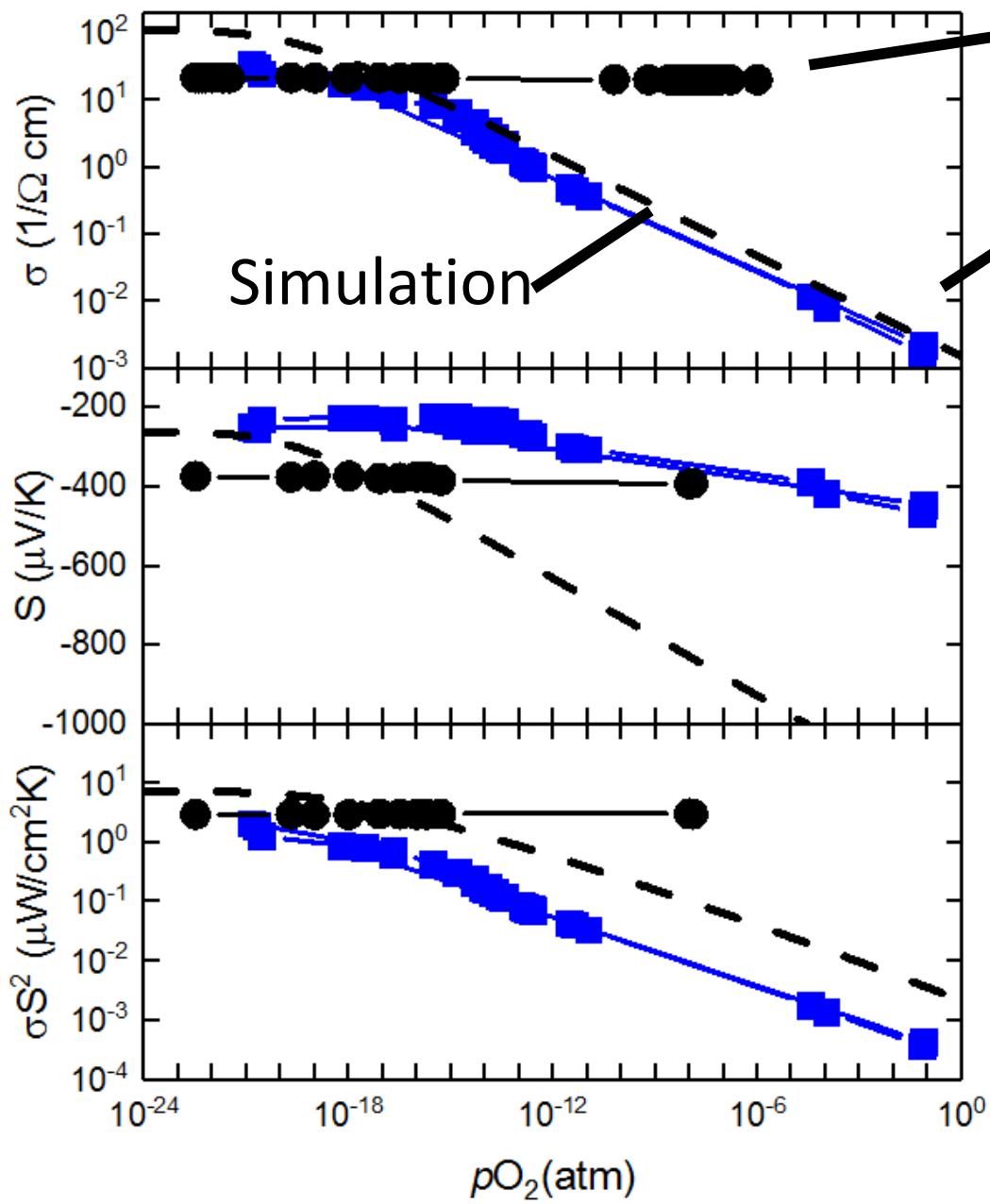
Hard to reach equilibrium even at 1 day
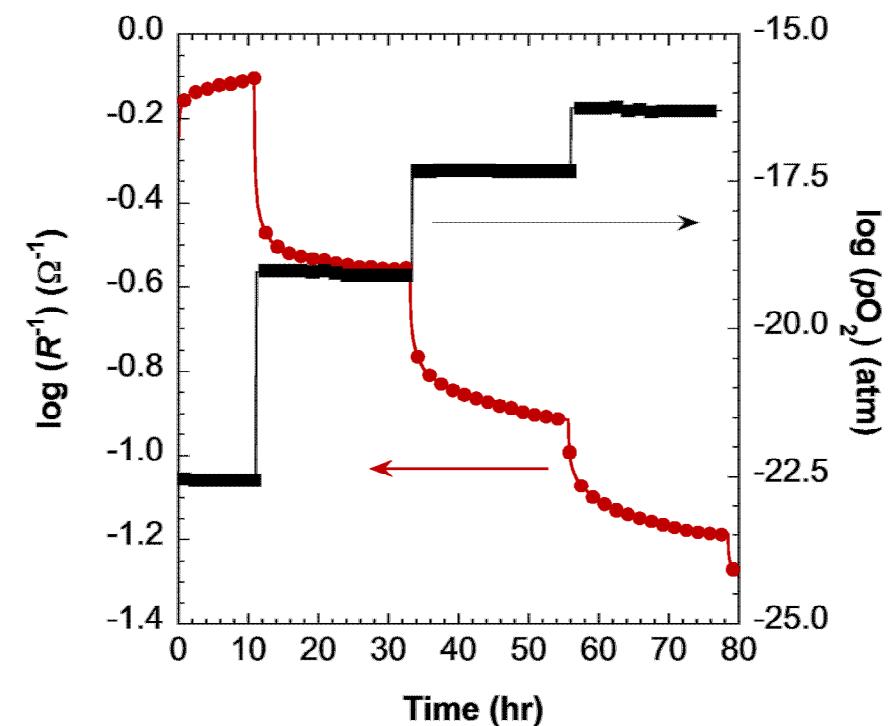
T = 1173 K
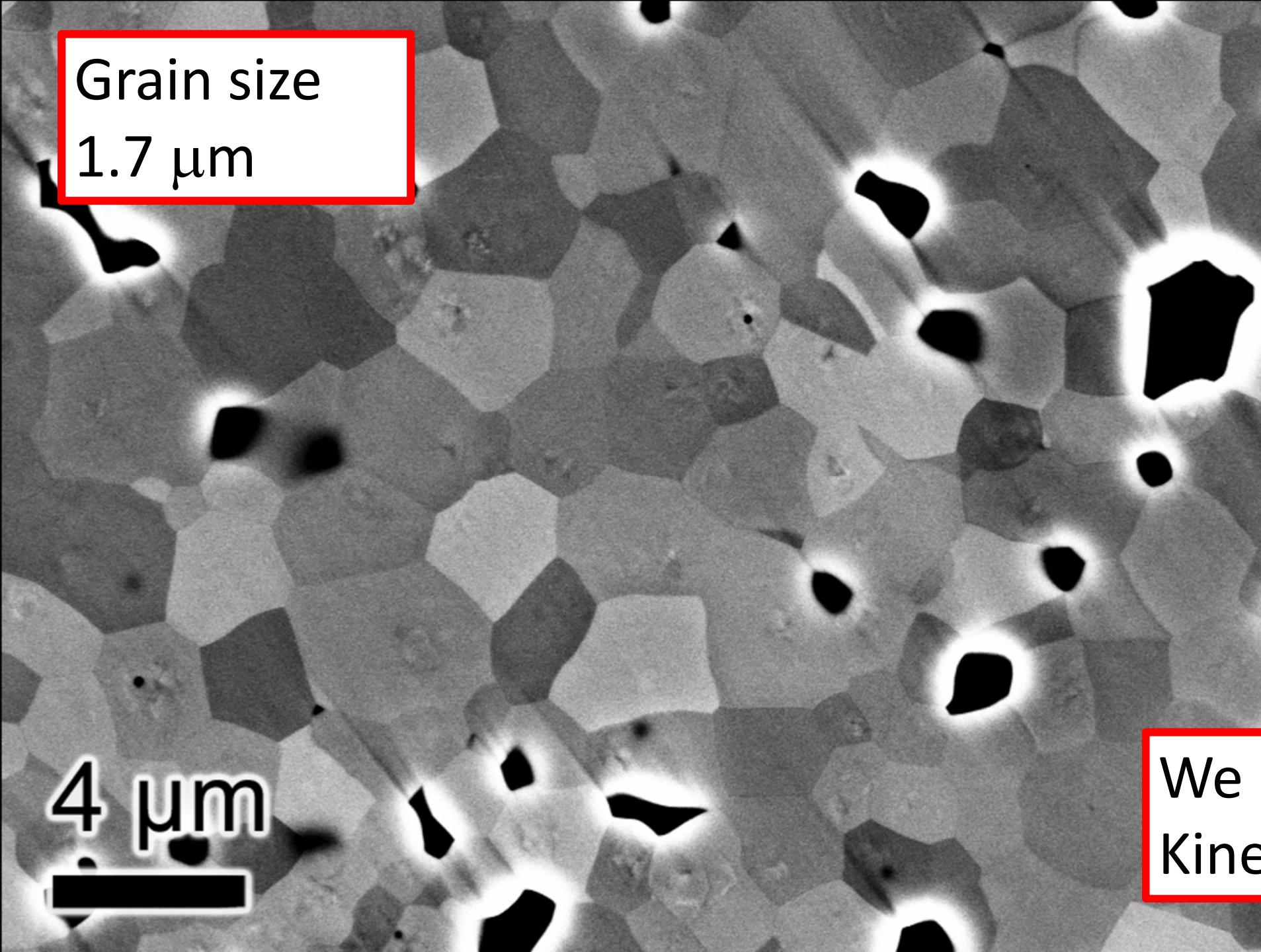
Grain size
1.7 µm

4 µm

Kinetics for Xtal
Versus Ceramic will be
different due to
Grain boundaries, pores

We need to know
Kinetics too

Oxidation of Donor doped $SrTiO_3$: Sr vacancy migration is rate-limiting step
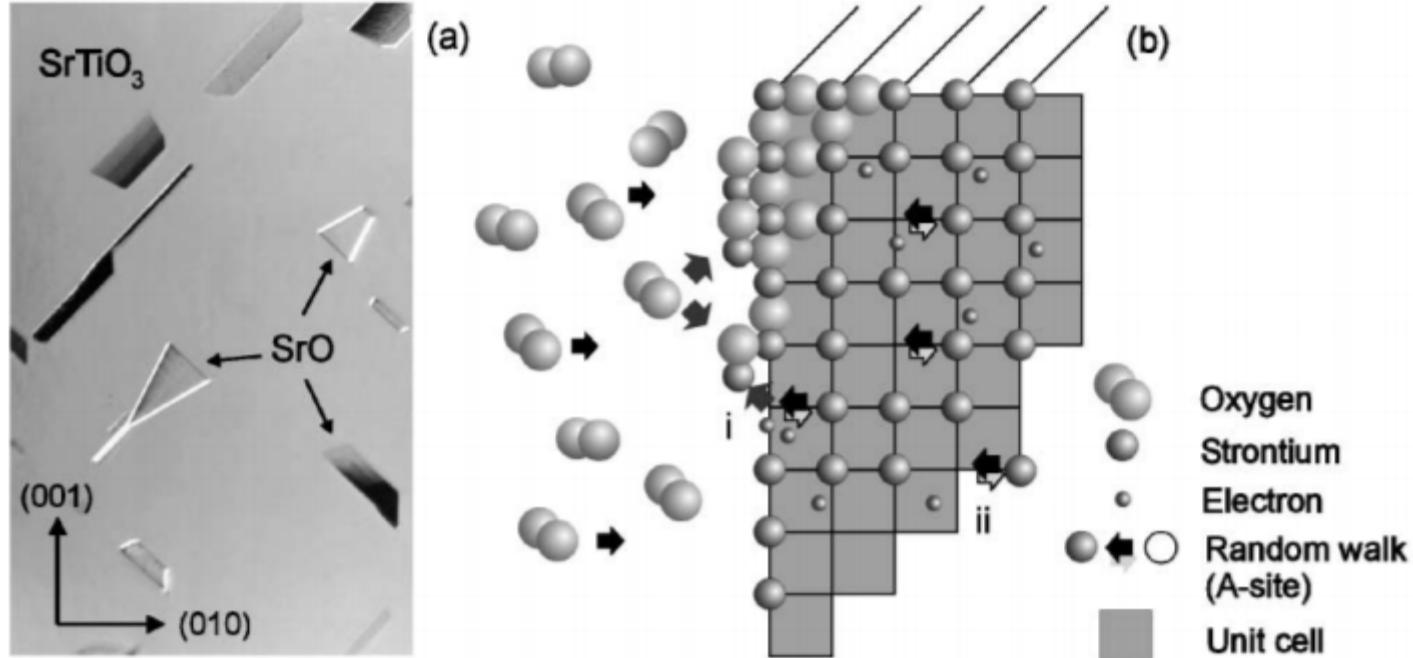
Meyer et al. PRL (2003)
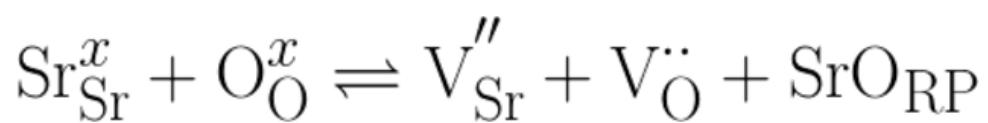
$$D \sim 1 \times 10^{-19} \mathrm{cm}^2/\mathrm{s}$$

T = 1173 K

Single xtal Nb doped $SrTiO_3$

$$Sr_{Sr}^x + O_O^x \rightleftharpoons V_{Sr}'' + V_O^{\cdot\cdot} + SrO_{RP}$$
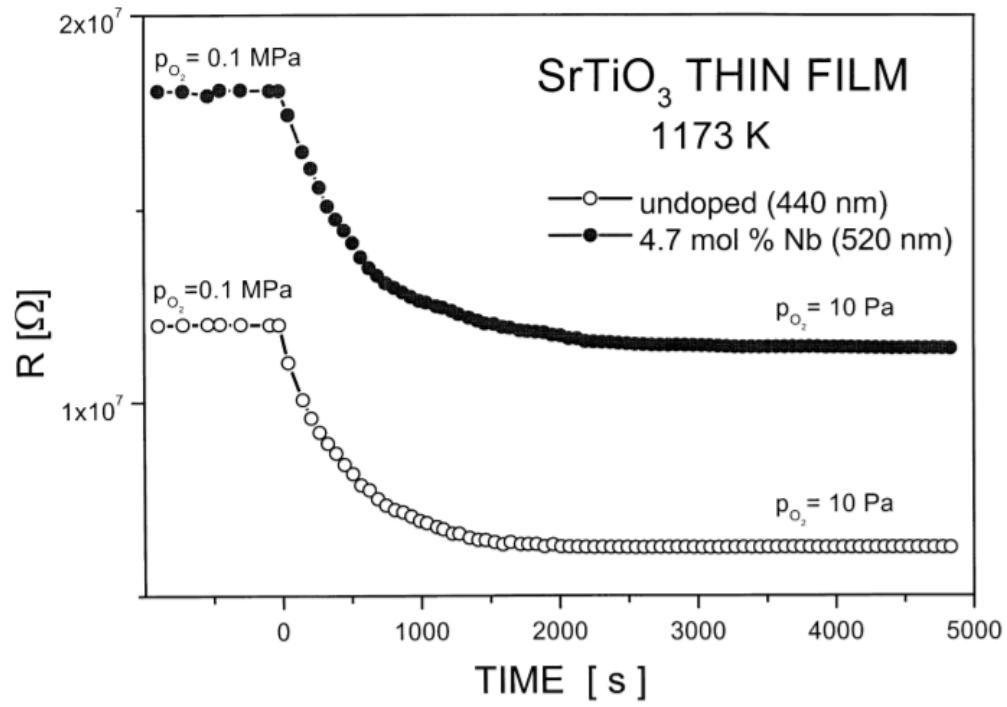
Pasierb et al. JPCS 1999

$$D \sim 1 \times 10^{-12} \mathrm{cm}^2/\mathrm{s}$$

$T = 1173$ K

Ceramic Nb doped SrTiO$_3$

Diffusion enhanced at grain boundaries
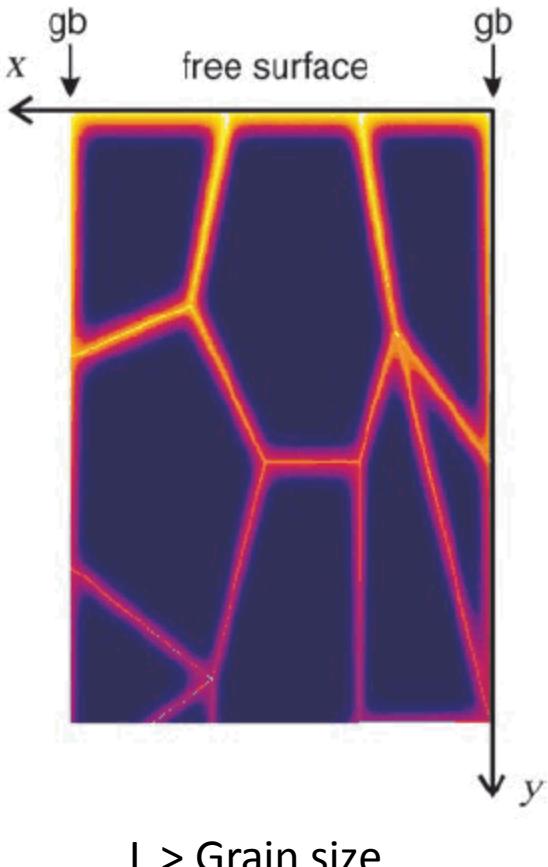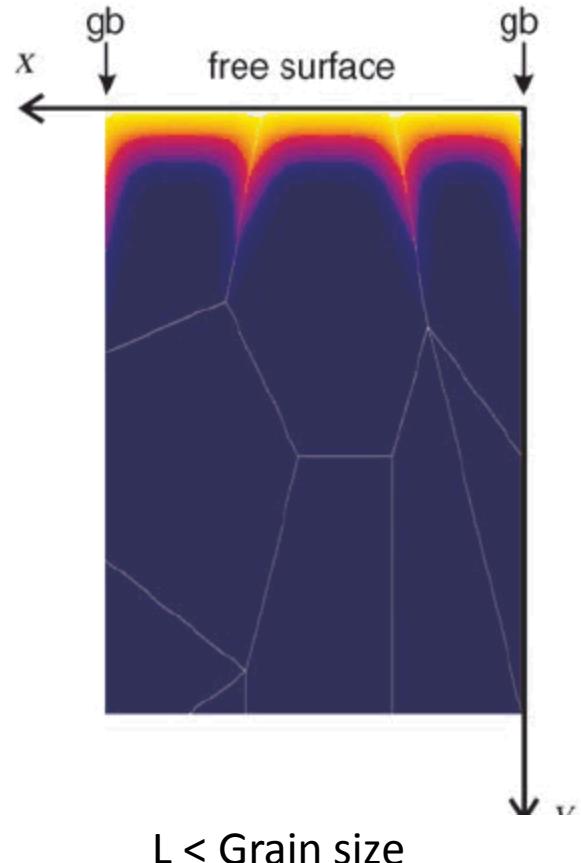
Grain size ~ 2 μm
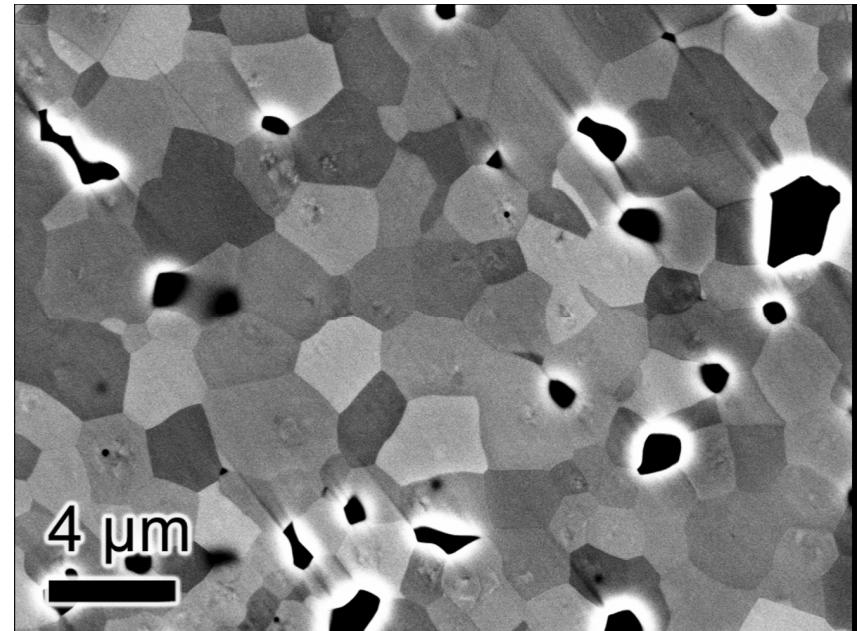
4 μm

$$L \sim \sqrt{Dt}$$

Material	24 hours	20 years
Ceramic	400 μm	3.5 cm
Xtal	0.3 μm	24 μm
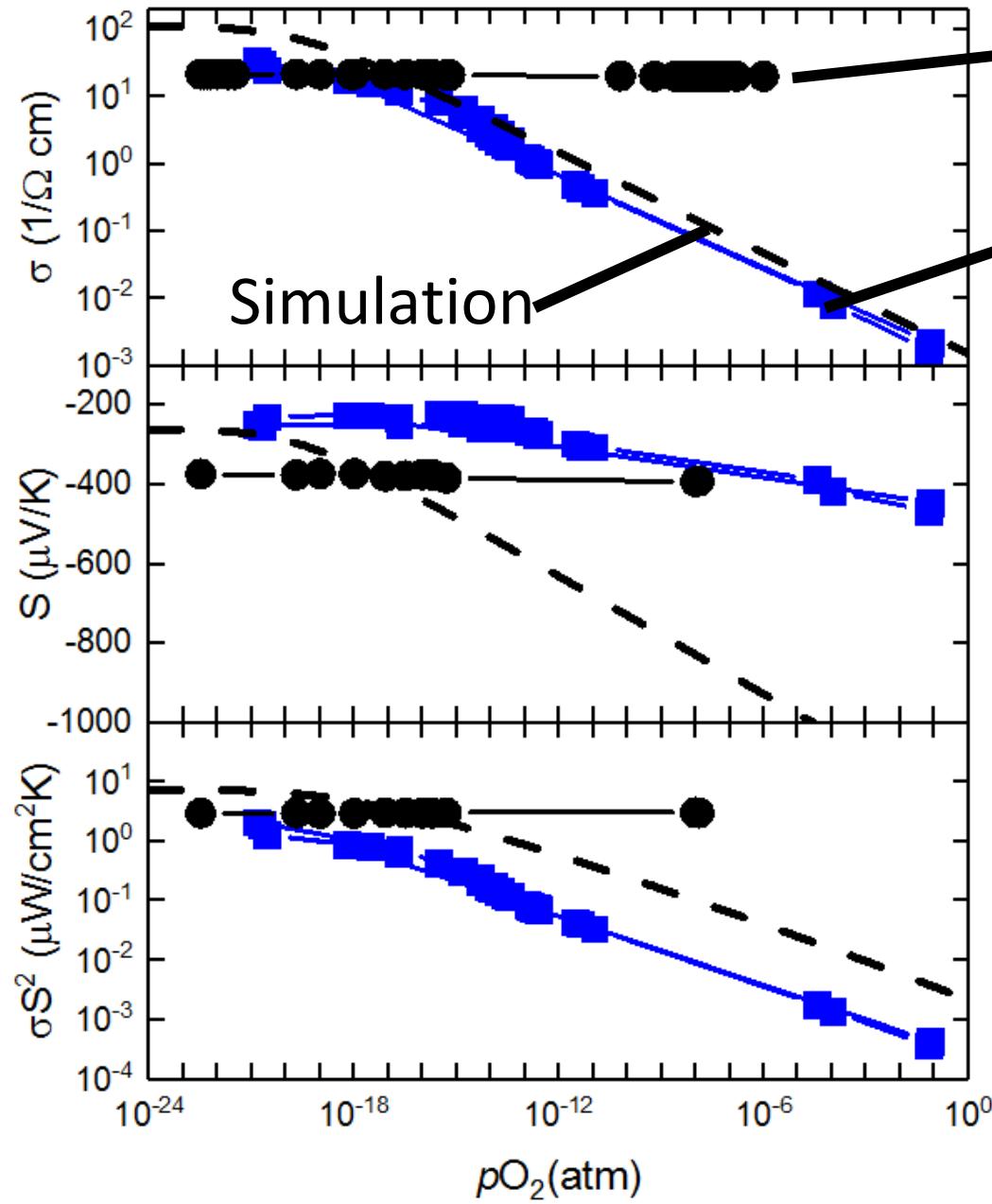
L < Grain size

L > Grain size

Merkle, Maier, Angew. Chem. 2008

σ (1/Ω cm)

Xtal 1% Nb-SrTiO$_3$

Simulation

Ceramic 10% Nb-SrTiO$_3$

Grain size ~ 2 μm

S (μV/K)

σS^2 (μW/cm^{2}K)

pO_2(atm)

x ← gb   free surface   gb →

y ↓

$$L \sim \sqrt{Dt}$$

Material	24 hours	20 years
Ceramic	400 μm	3.5 cm
Xtal	0.3 μm	24 μm

Xtal 1% Nb-SrTiO$_3$

Ceramic 10% Nb-SrTiO$_3$

Simulation
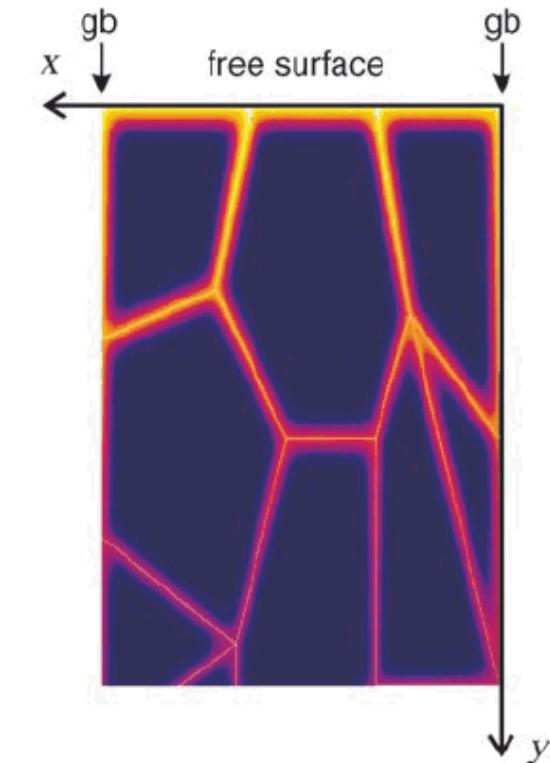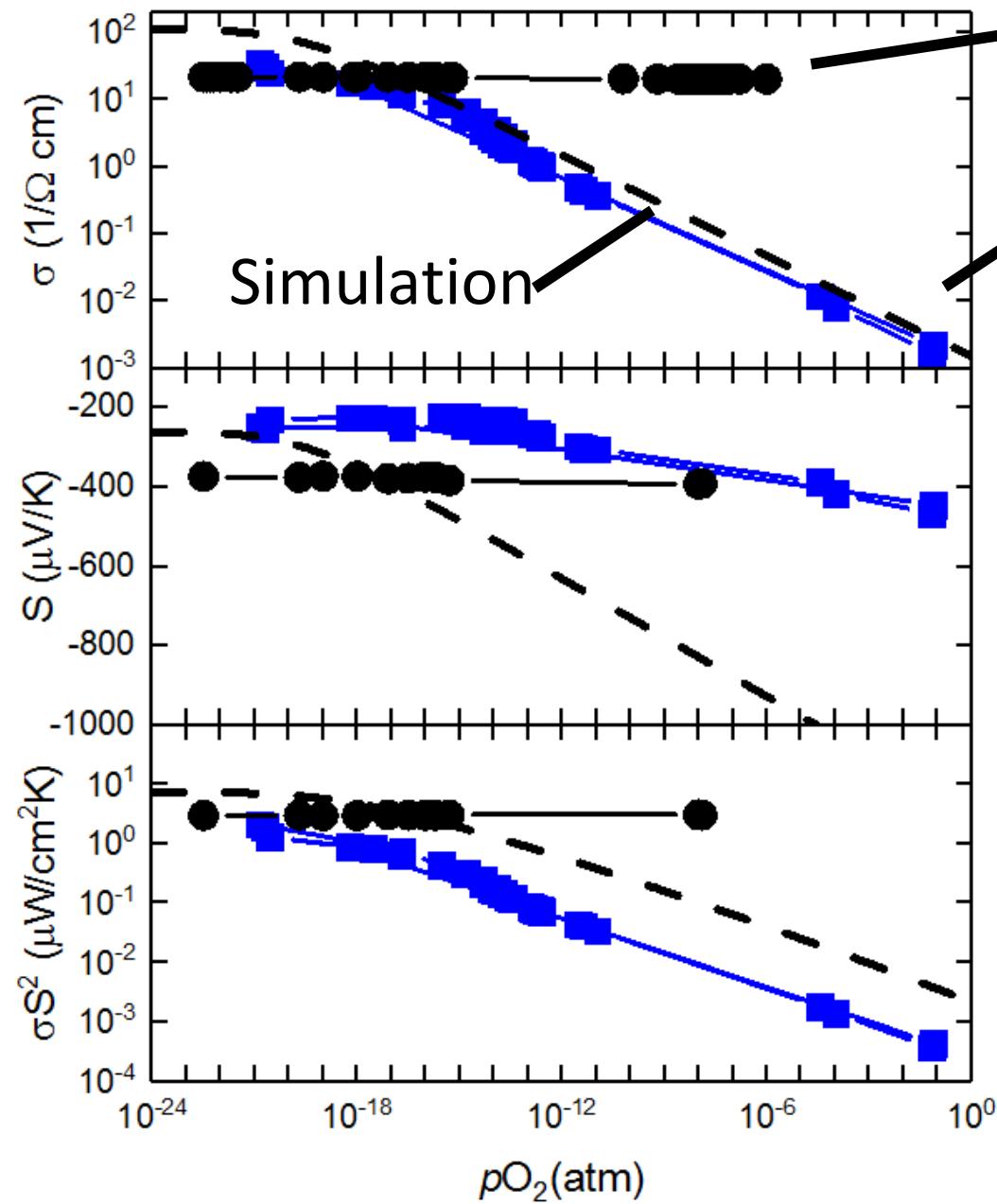
Single Xtals are stable in air

Ceramic samples are not

Not easy to use single crystals in actual applications

"Nanostructuring" can be incompatible with stability in air...

SrTiO$_3$

Wang et al. APX 2010
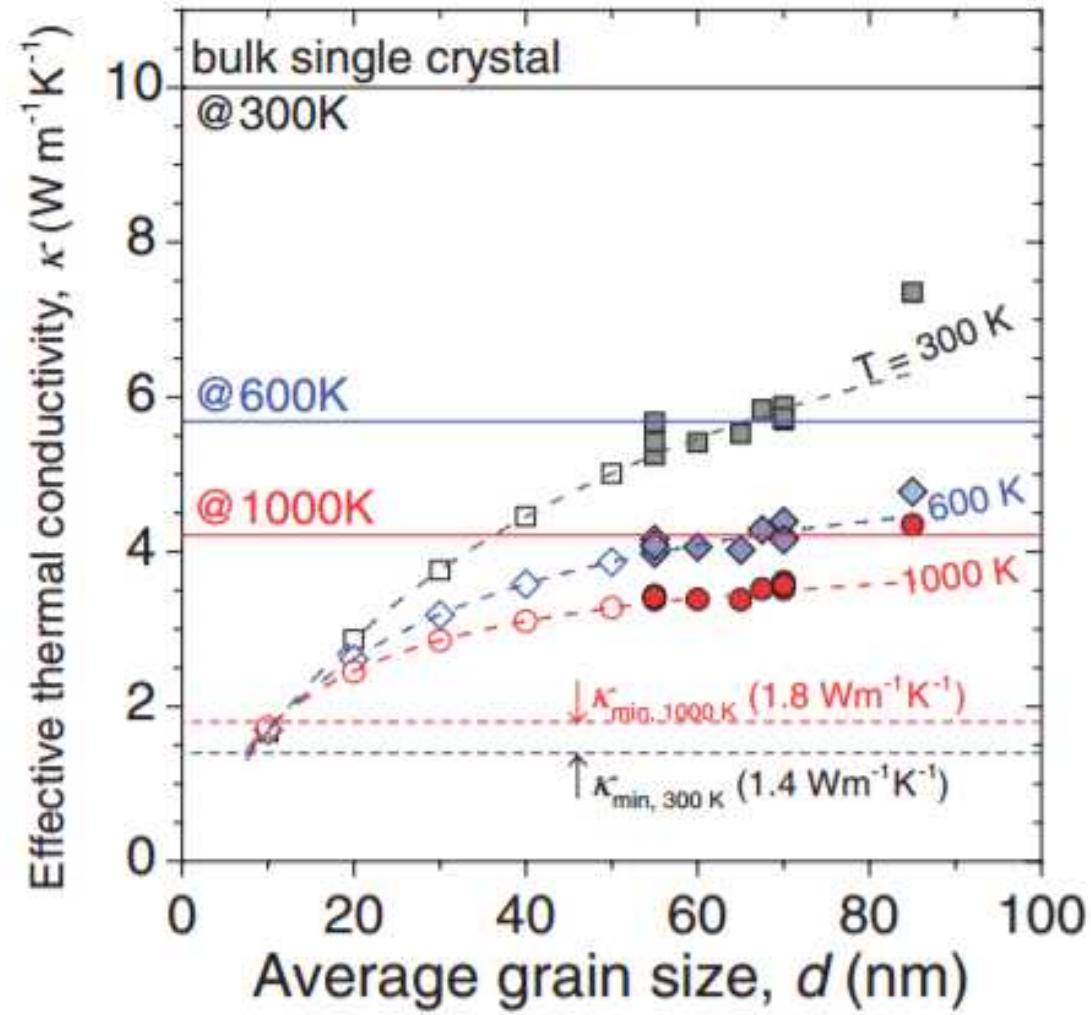
Are thermoelectric oxides "stable in air"?

Yes and No

In equilibrium, oxides are not *a priori* more or less stable than non-oxides

You need to take into account defect equilibria and kinetics

Temperature matters too.
T<900 K defect kinetics slow down a lot for $SrTiO_3$
(but efficiency is lower)

Other consequences

Are P and N oxides stable under the same conditions at the same temperatures with the desired ZT?

Interaction of oxide thermoelectrics with other oxygen-containing materials at the module/systems level?

No clear benefit for systems complexity in general

Xtal 1% Nb-SrTiO$_3$

Ceramic 10% Nb-SrTiO$_3$
Grain size ~ 2 μm

Simulation
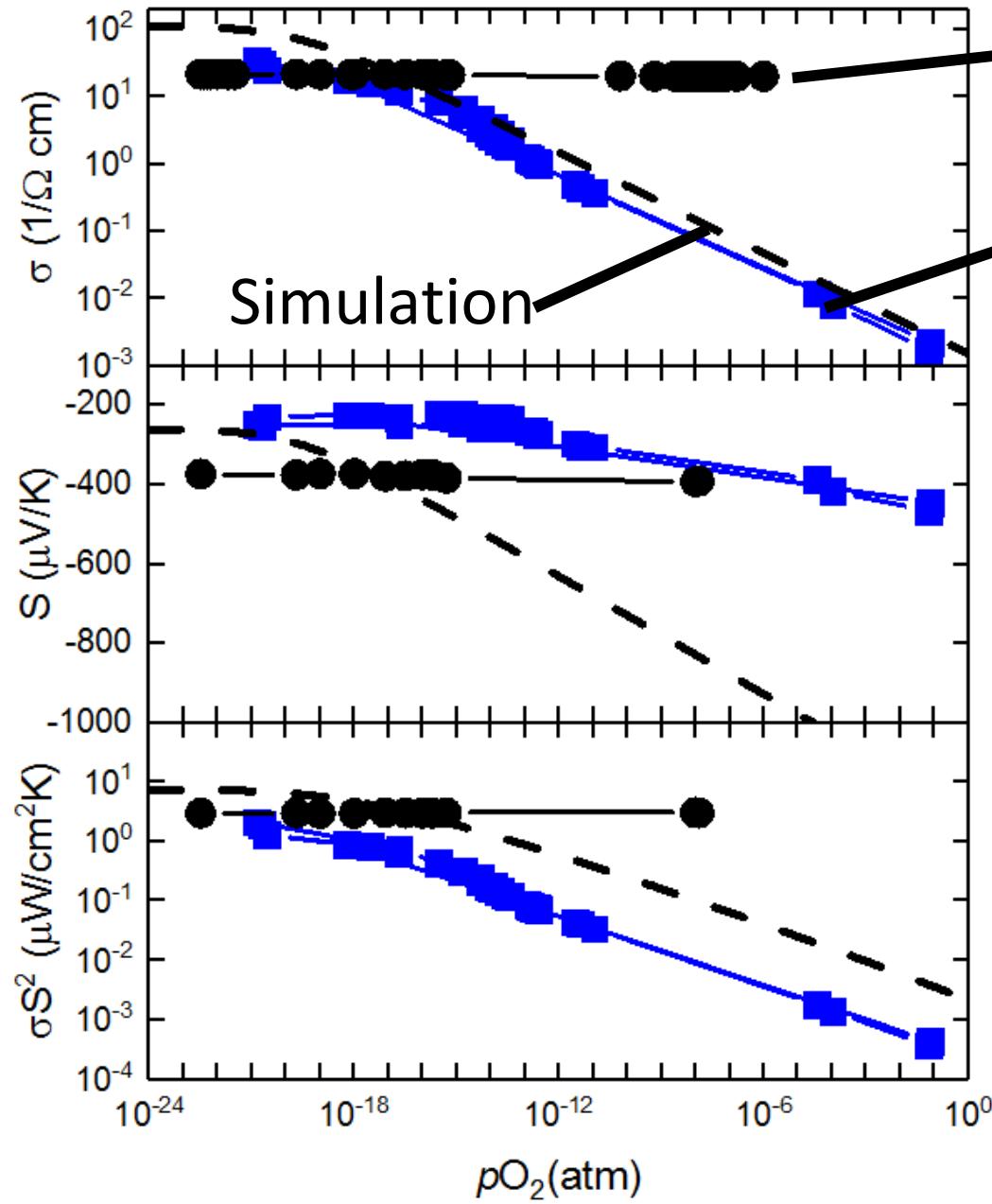
Donor doped SrTiO3 will be challenging to use in air environments in ceramic form.

What are the defect reactions and kinetics relevant for other popular oxide materials?