ION IMPLANTATION TO CONTROL THE THERMOELECTRIC PROPERTIES OF THIN FILMS

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Context

Ion implantation as a strategy to improve thermoelectric properties:

↓

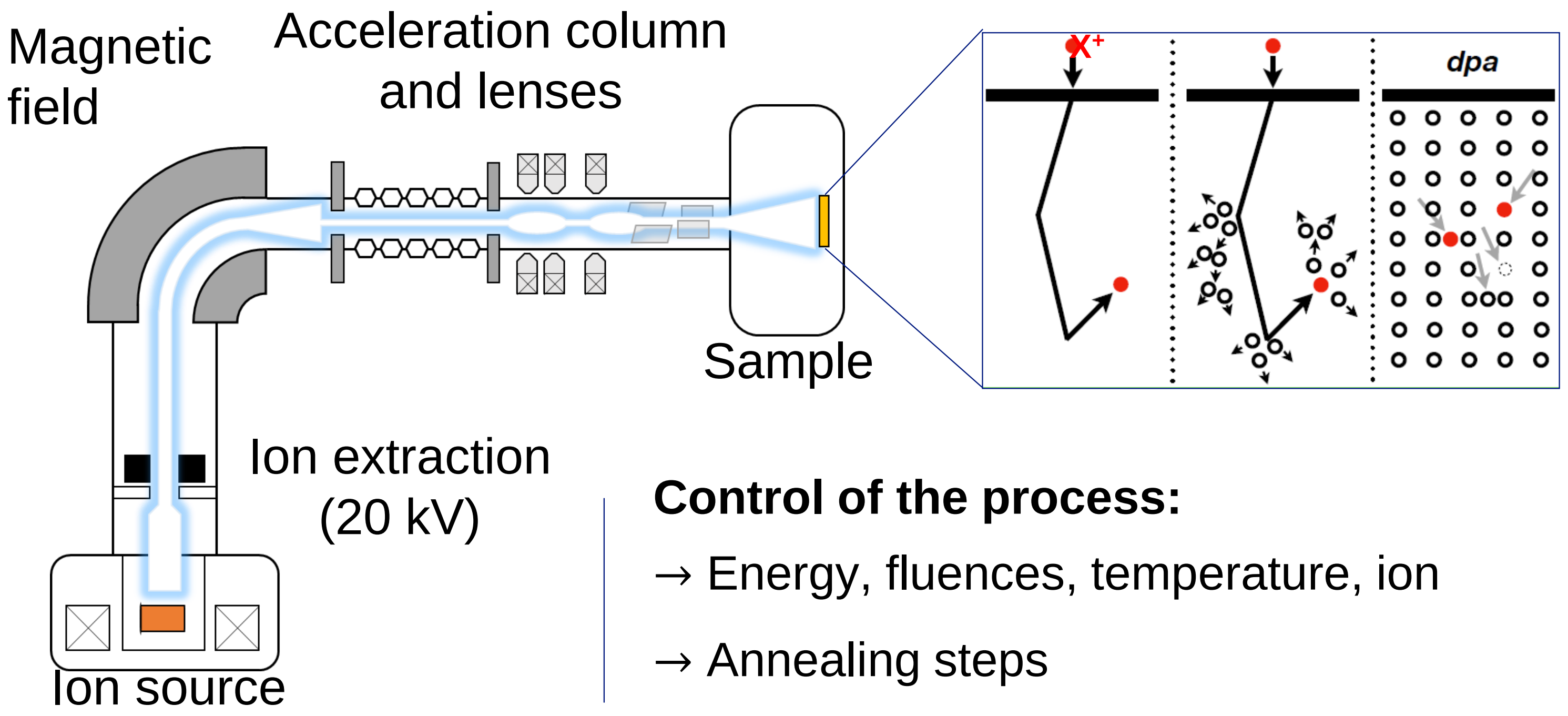
Engineering of defects: Electrically active (doping) or not

↙ ↘

Optimization of carrier concentration

Reduction of thermal conductivity

Ion implantation



Control of the process:

→ Energy, fluences, temperature, ion

→ Annealing steps

Why Scandium Nitride (ScN)?

- ➕ High Power factor: ~3 $mW.m^{-1}.K^{-2}$ [1] ⇒ n-type degenerate semi-conductor
- ➖ High thermal conductivity: ~12 $W.m^{-1}.K^{-1}$

↪ due to oxygen incorporation [2]

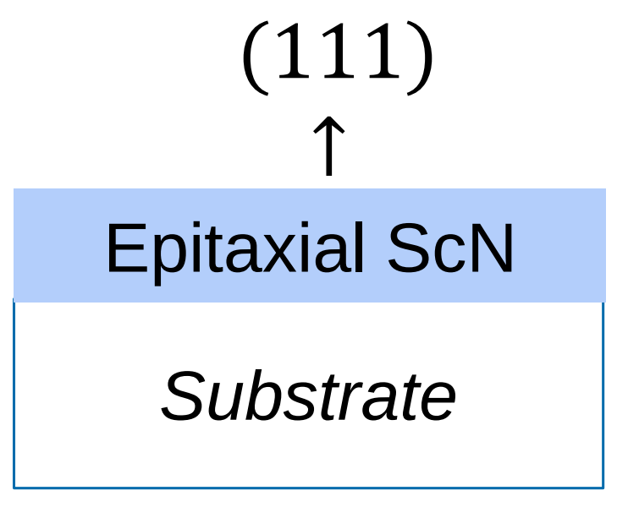
→ O_N is donor defect [2]

Previous work on ScN: Mg^+, Li^+ and Ar^+ [4,5,6]

→ $\boldsymbol{\kappa}$ decreased to 2 – 7 $W.m^{-1}.K^{-1}$ = **phonon scattering increased**

→ S increased but σ decreased = **DOS modified and carriers trapped**

ScN thin films



↕ 220 nm

Al_2O_3 c-cut or MgO (111)

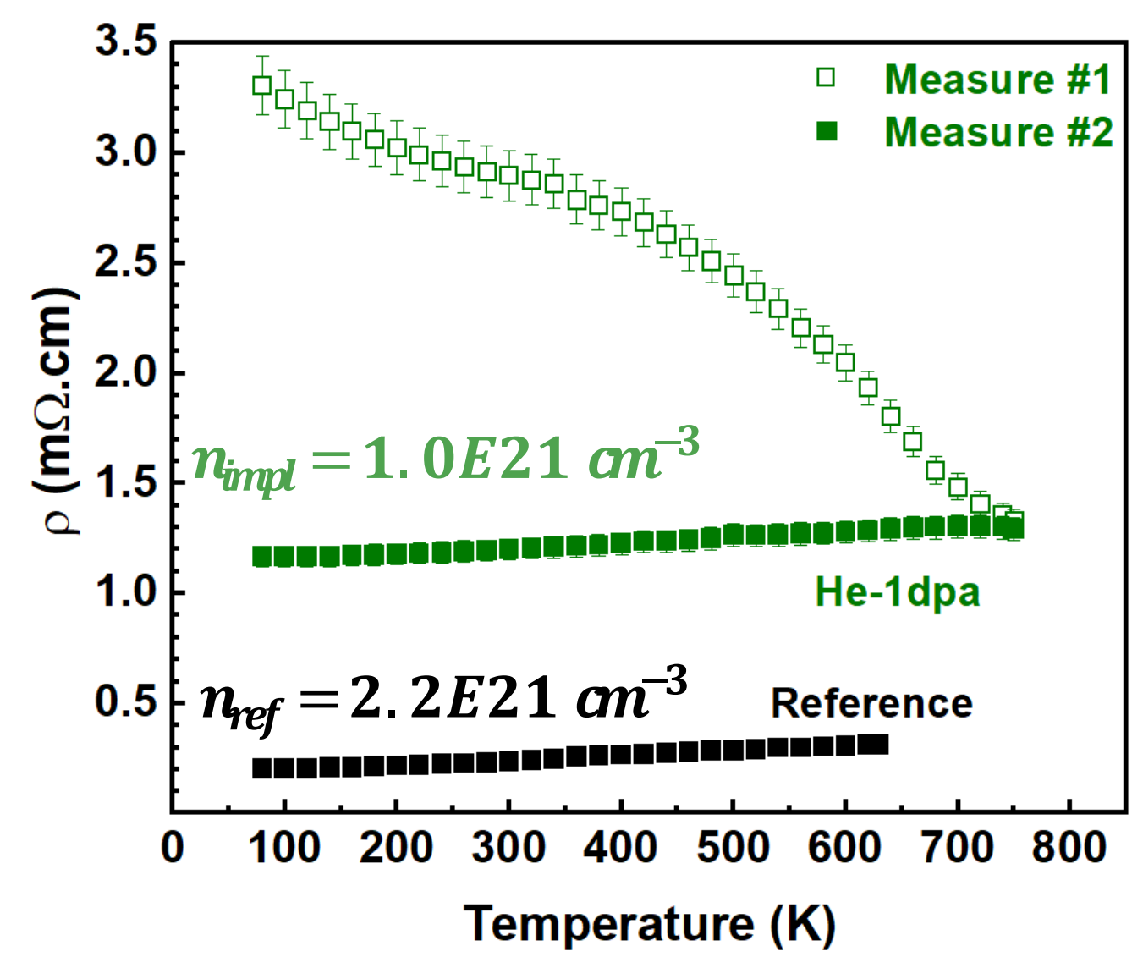
- Magnetron sputtering deposition
- NaCl type structure

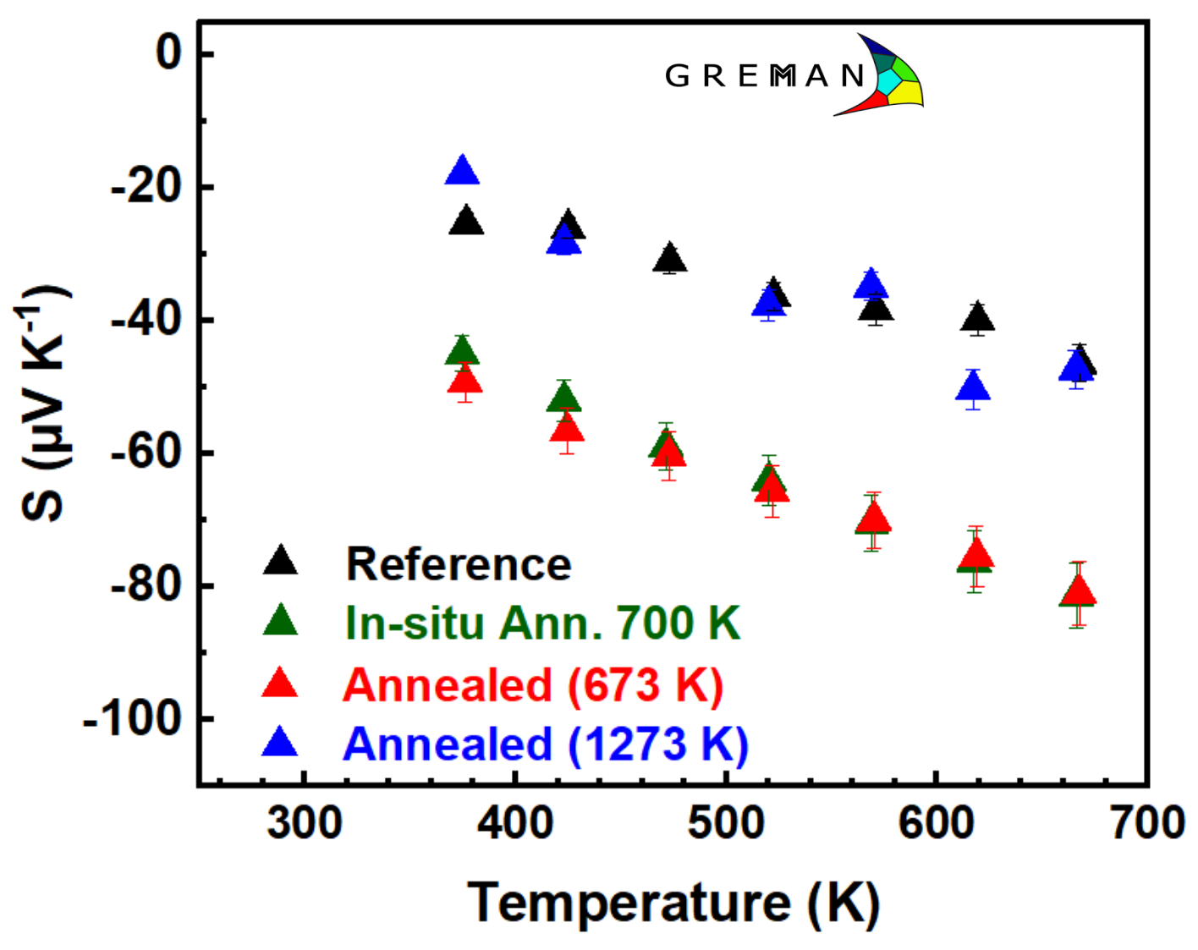
- $n = 2.2 \pm 0.2 \times 10^{21}\ cm^{-3}$
- $\rho_{300K} = 0.06\ to\ 0.2\ m\Omega.cm$
- $\mu_{300K} = 10\ to\ 40\ cm^2.V^{-1}.s^{-1}$
- $S_{300K} = -20 \pm 5\ \mu V.K^{-1}$

Results and Discussions

dpa = displacement per atom

HELIUM 1dpa





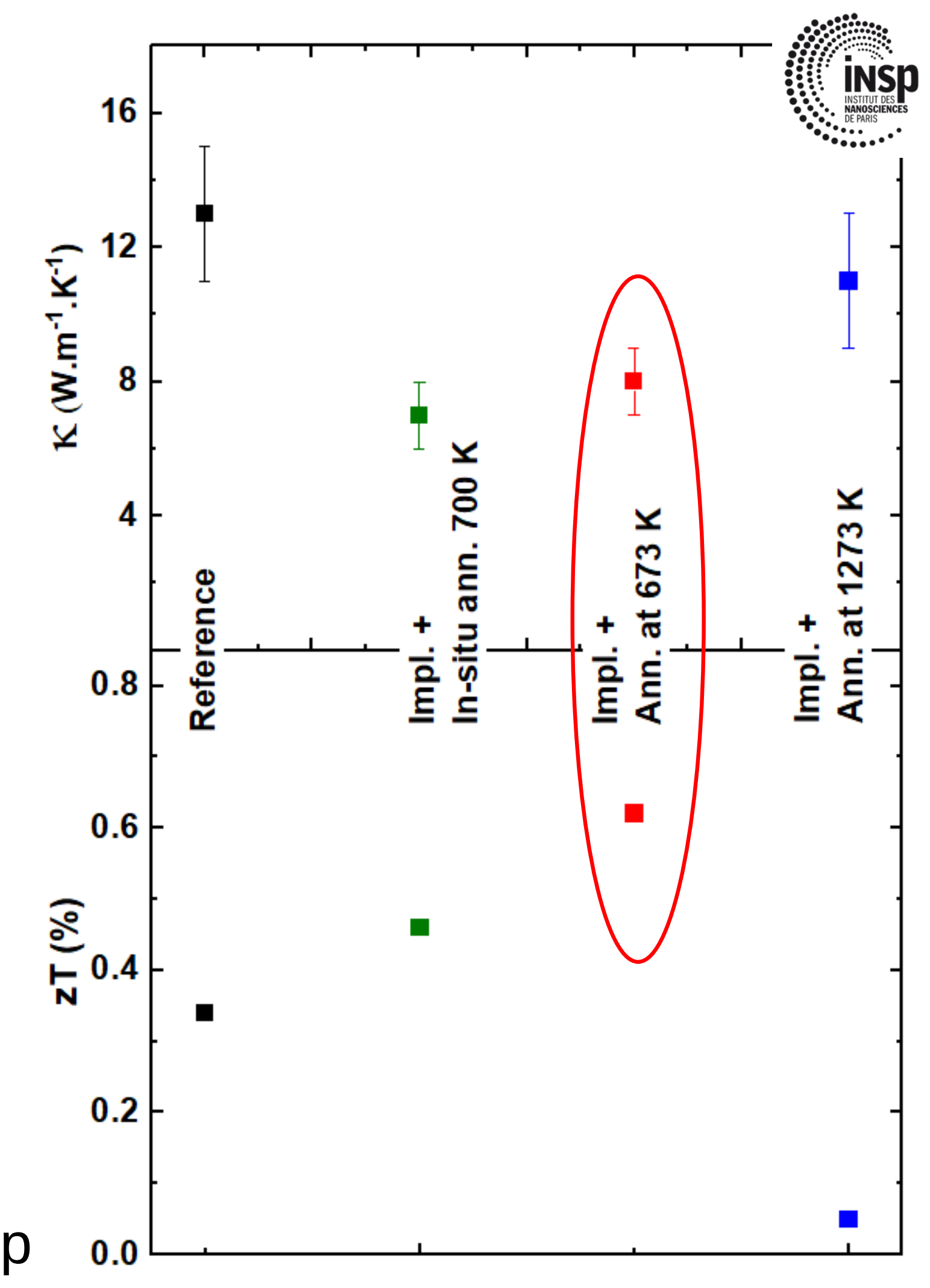
- ❑ **Defect generated:** Electrically not active → From ballistic effect

❖ **Point-like defects**

- Induce **localized states** near Fermi level → electrical conduction mechanism modified
- Fully recombined at 700 K

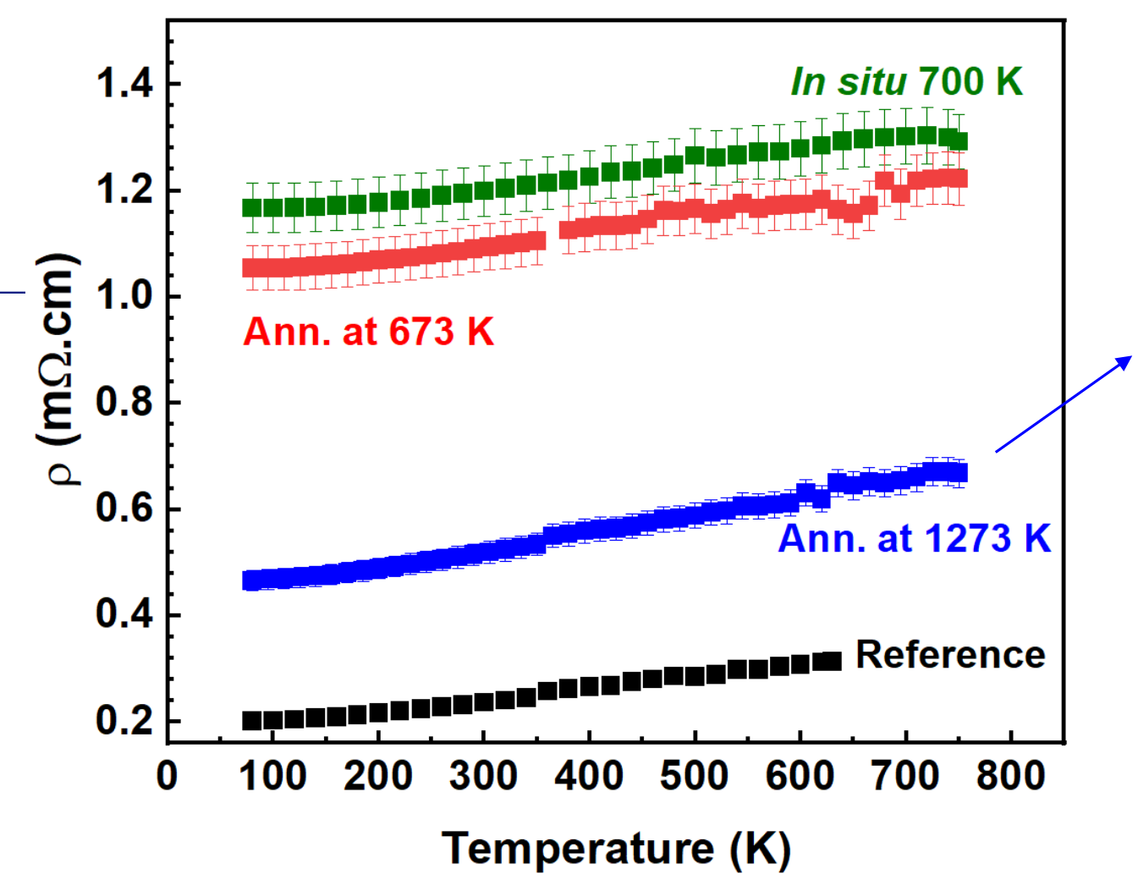
❖ **Complex-like defects**

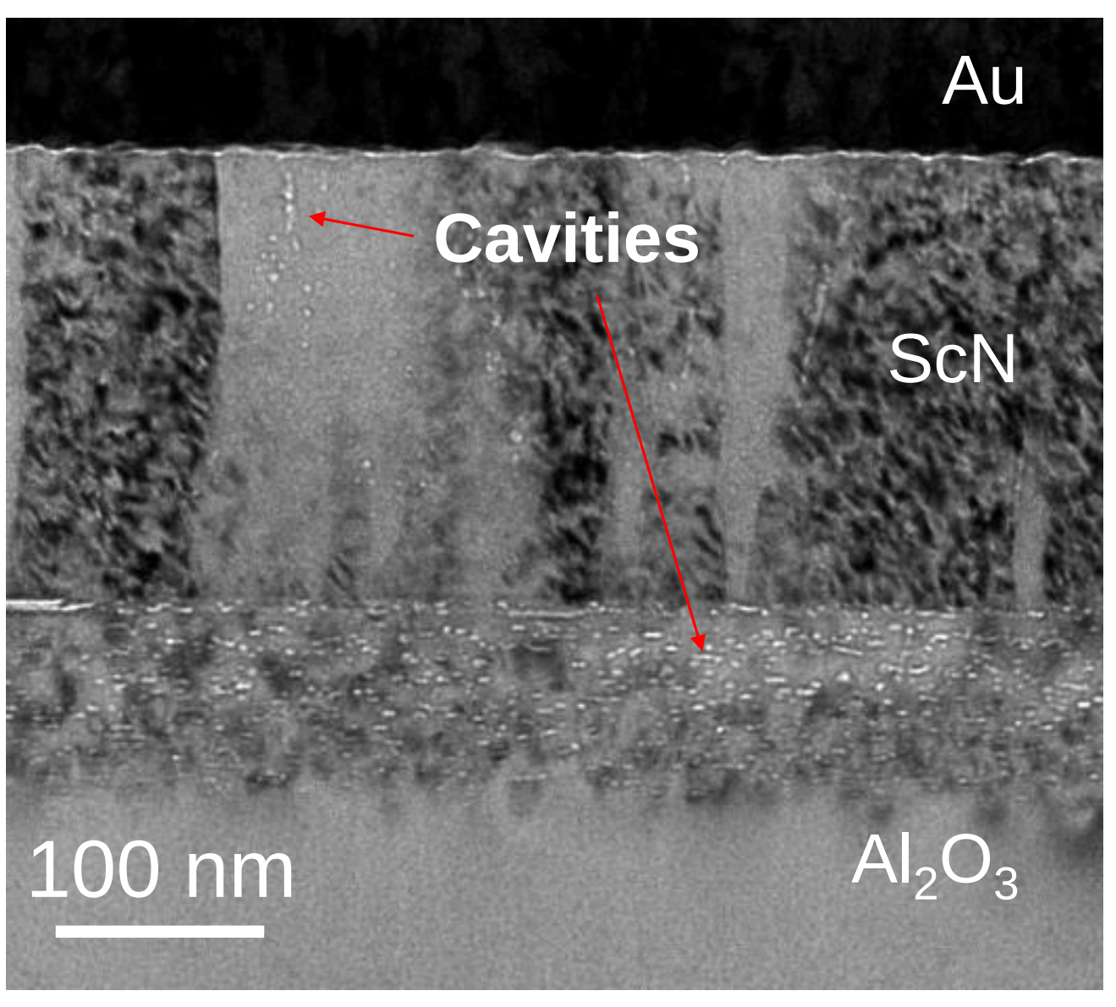
- **Deep acceptor level** in the band gap → trapping of carriers + scattering centers



- ❑ **Recombination of the defects**:
- Partial recovery of all properties

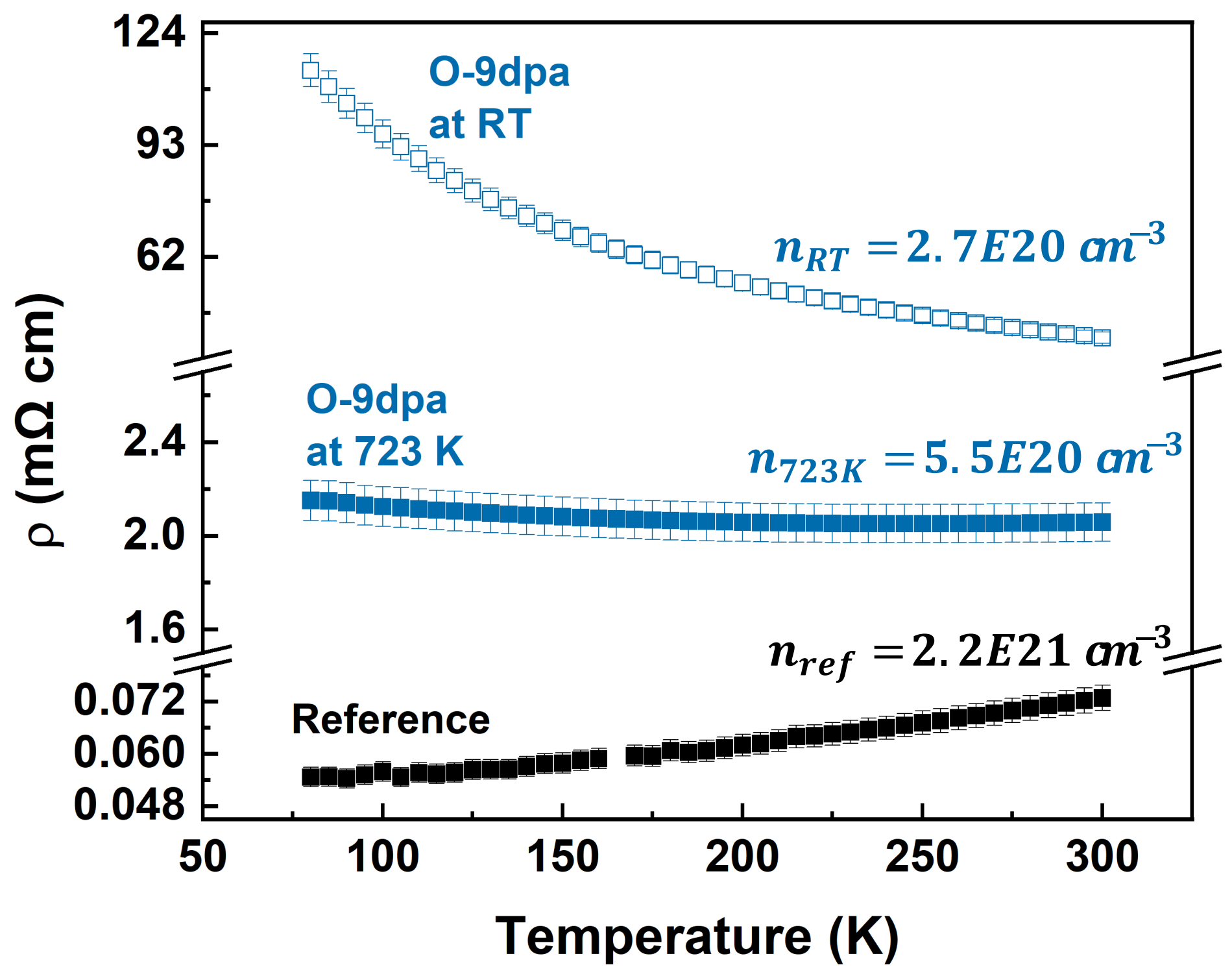
→ Remaining defects after high temperature annealing





He-implanted ScN film and annealed at 1273 K

OXYGEN 9dpa



- Same behavior as He: change in conduction mode + trapping of carriers
- Higher magnitude = more defects created

→ **Acceptor defects** with higher formation energies (O_i, V_{Sc} complexes…)

→ Not only ballistic effect: also chemical effect

Conclusion and Outlooks

- ❑ Complex-like defects: stable up to 750 K→ acts as scattering centers + carriers traps
- ❑ Evolution of defects → cluster to cavities
- ❑ **Successful increase of zT by reducing $\boldsymbol{\kappa}$** → optimization TE properties with defects

- ❑ Optimization on oxygen implantation and understanding of defects induced
- ❑ Effect of initial doping of ScN

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