



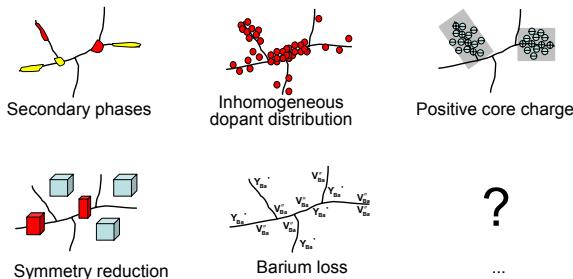
Space charge effect and dopant segregation in acceptor-doped BaZrO_3 proton conductors

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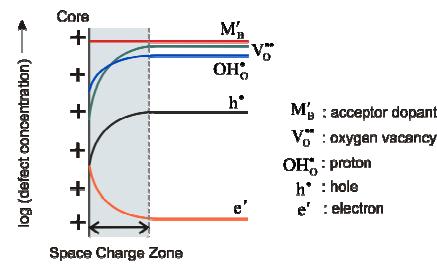
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- Potential reasons for blocking grain boundaries (GBs)



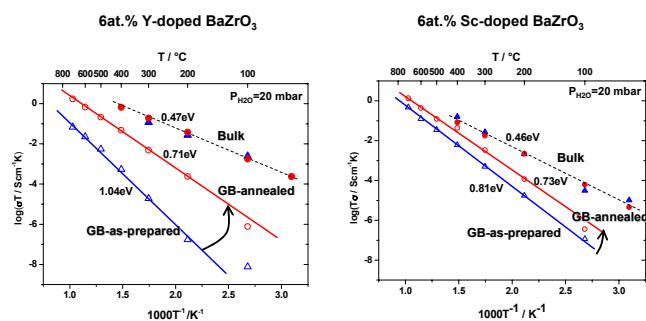
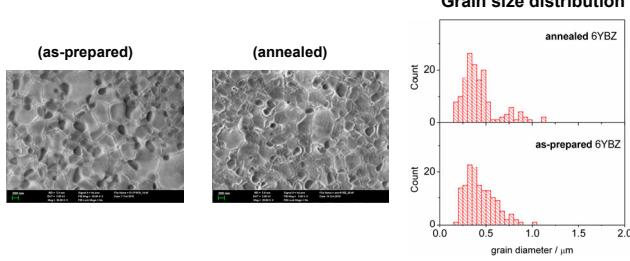
- Blocking effect at the GB and space charge model:



I) High temperature annealing

- **As-prepared sample:** Spark Plasma Sintered (SPS) at 1600°C / 5 min / 50 MPa
 - **Annealed sample:** SPS sample annealed at 1700°C / 20 h $\rho \approx 98\% \rho_{th}$

No grain growth during annealing

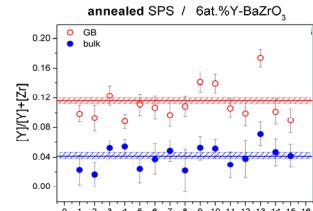
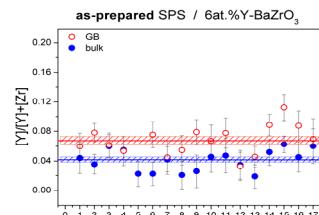
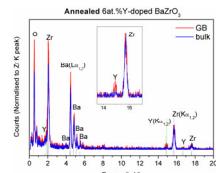
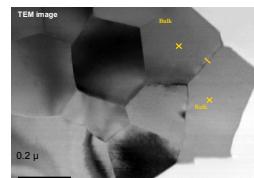


annealing: dopant segregation to
GB core and space charge zone
⇒ decreased proton depletion
in space charge zone

- Same σ_{H^+} for bulk, strongly increased σ_{H^+} for GB
- Lower space charge potential
- Comparable effect for Y- and Sc-doped BaZrO₃

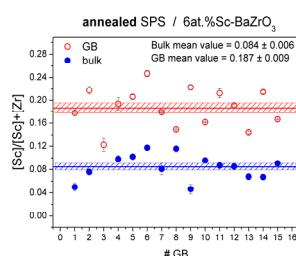
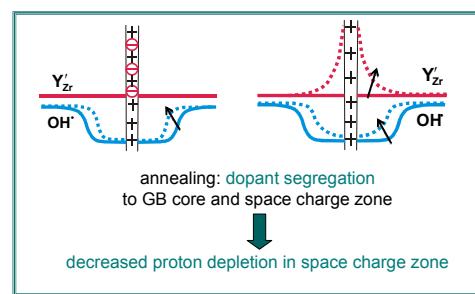
II) Dopant segregation

GB composition by EDXS-TEM



as-prepared:
slight Y excess at GB

annealed:
strong Y segregation to GB region



Sc³⁺ GB excess \approx Y³⁺ GB excess
 $(r = 0.72 \text{ \AA})$ $(r = 0.90 \text{ \AA})$

 electrostatic driving force dominates
 over elastic contribution