Atomic-scale origin of the low grain-boundary resistance in perovskite solid electrolyte $Li_{0.375}Sr_{0.4375}Ta_{0.75}Zr_{0.25}O_3$

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The **main achievement** of this research is revealing the atomic-scale origin of the low grain-boundary (GB) resistance in $Li_{0.375}Sr_{0.4375}Ta_{0.75}Zr_{0.25}O_3$ (LSTZ0.75) perovskite solid electrolyte and providing insights on overcoming the ubiquitous bottleneck of high GB resistance in other oxide solid electrolytes.

Significance of this scientific achievement

· Aberration-corrected scanning transmission electron microscopy and spectroscopy, along with an active learning moment tensor potential, were used to reveal the atomic scale structure and composition of LSTZ0.75 GBs.

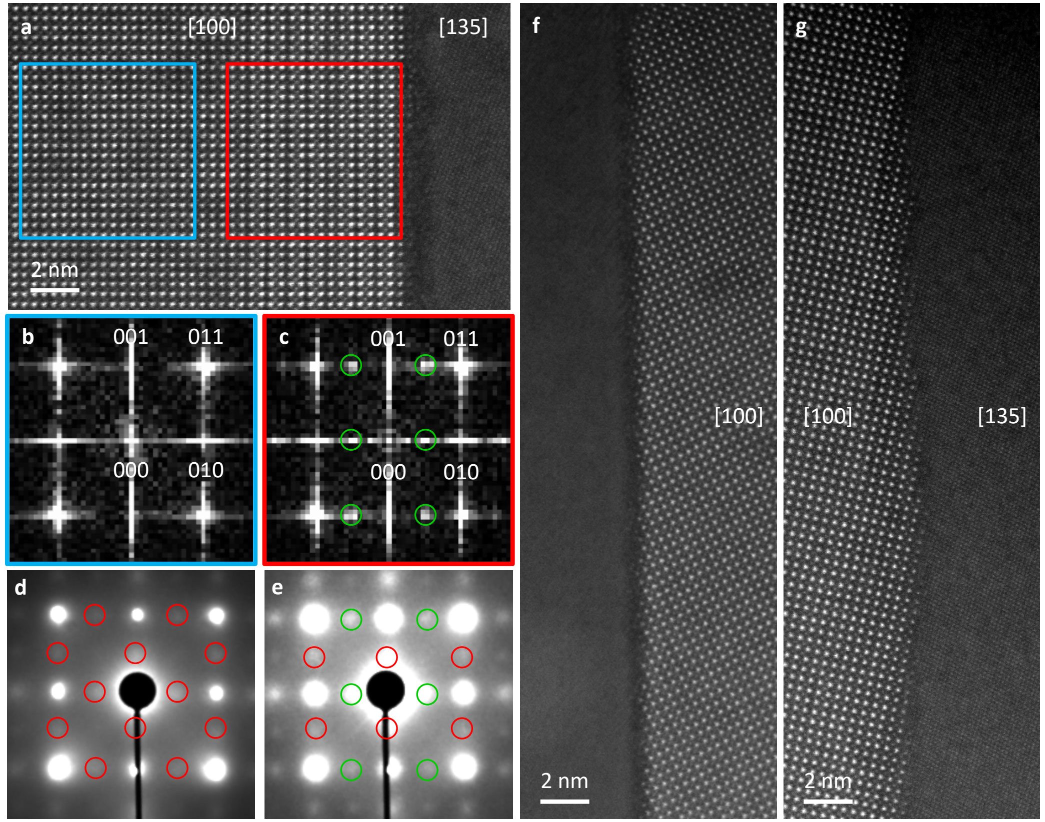
· Li depletion, which is a major cause for the low GB ionic conductivity of $Li_{3x}La_{2/3-x}TiO_3$ (LLTO), was found to be absent for the GBs of LSTZ0.75.

· A unique defective cubic perovskite interfacial structure that contained abundant vacancies was discovered at the GBs of LSTZ0.75. The authors attributed the low GB resistance of LSTZ0.75 to this microstructure.

· Based on these results, the authors conclude vacancy and defect engineering can effectively improve GB ionic conductivity of solid Li-ion conductors, given that the material's original structural framework should be maintained.

Contribution to IRG 1

This study provides new insights into the atomic-scale mechanisms of low GB resistance and sheds light on possible paths for designing compositionally complex oxide solid electrolytes with high total ionic conductivity.



Atomic-scale study of the crystal structure inside the grain bulk, a (010) faceted grain boundary (GB), and non-faceted general GBs.

Lee T, Qi J, Gadre CA, Huyan H, Ko S-T, Zuo Y, Du C, Li J, Aoki T, **Wu R, Luo J, Ong SP, Pan X**. "Atomic-scale origin of the low grain-boundary resistance in perovskite solid electrolyte $Li_{0.375}Sr_{0.4375}Ta_{0.75}Zr_{0.25}O_3$". *Nature Communications*, **14**, 1940 (2023). https://doi.org/10.1038/s41467-023-37115-6