Modeling of New Materials for Solid Oxide Cells

Scaling Hydrogen Production through Accelerated Ion Transport

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Introduction

New ways of producing alternative energy or improving existing energy technologies that can store renewable energy is paramount to achieving the net-zero emission target.

The electrolyte layer of solid oxide cells has mostly been constructed using oxide ion conductors and enhancing these materials have the potential of improving energy conversion efficiency.

Innovation and Objectives

The study proposes a novel method of enhancing ionic conductivity by applying strain in three dimensions by embedding nanoparticles in electrolyte materials.

- Build a computational strain-conductivity model.
- Experimentally develop novel ceramic-based electrolyte materials.

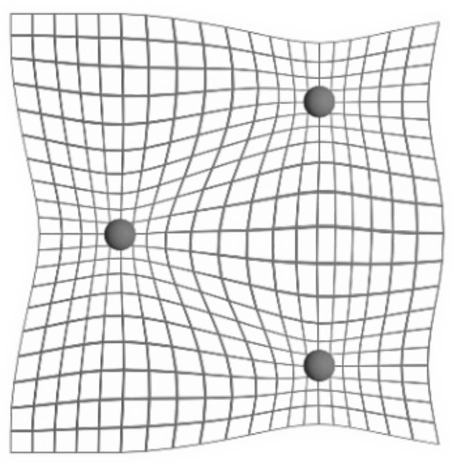

Figure 1. *Illustration of crystal lattice distortion.*

Modeling and Experimental Work

A voxel of 100 nm edge was used for computing particle spatial configurations. The average volumetric strain, ε_v, is computed with equation given by;

$$\overline{\varepsilon_V} = \frac{\sum_{i=1}^{n}\left(\frac{1}{LN}\overline{\varepsilon_L}_{LN=26}\right)_i}{n} \qquad (1)$$

Conductivity enhancement of the system is given by,

$$\frac{\overline{\sigma_{\varepsilon_V}}}{\sigma_0} \approx e^{\alpha\overline{\varepsilon_V}} \qquad (2)$$

In summary, the steps to model endo-particle system embedded with nanoparticles is highlighted below.

Spatial Configuration → Local Strain → Volumetric Strain → Ionic Conductivity

The experimental work for the preparation of the electrolyte material are as depicted in the pictures below.

Figure 2a. Sonication process

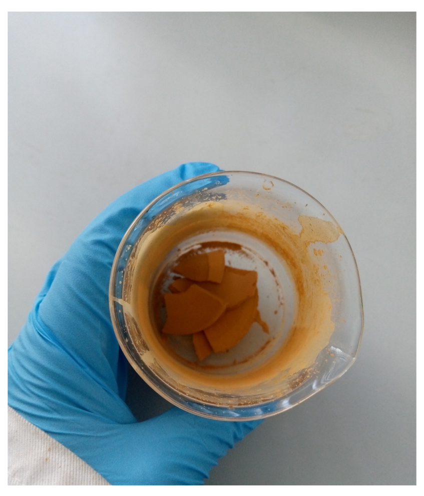

Figure 2c. Dried mixture after sonication

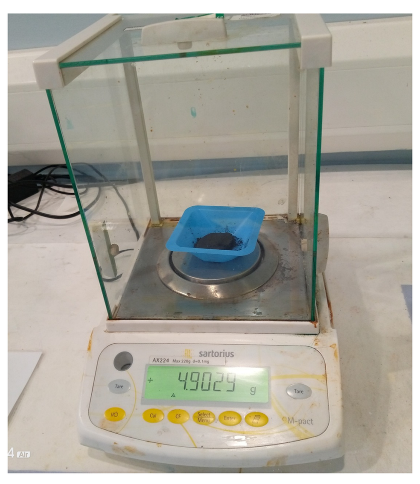

Figure 2e. Weighing the synthesized perovskite

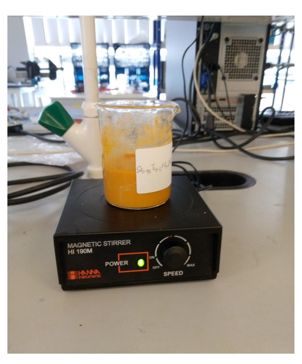

Figure 2b. Stirring the mixture

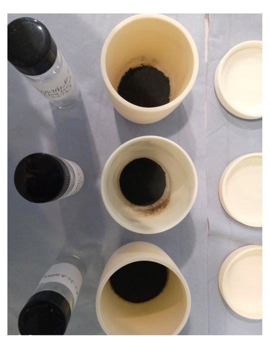

Figure 2d. Calcined perovskites

Figure 2f. XRD analysis

References

[1] Great Britain Department for Business, Energy & Industrial Strategy, *UK Hydrogen Strategy*. [London]: [Dandy Booksellers Ltd], 2021.
[2] K. Kousi, D. Neagu, L. Bekris, E. I. Papaioannou, I. S. Metcalfe, 2020, 6, 59

Results

a

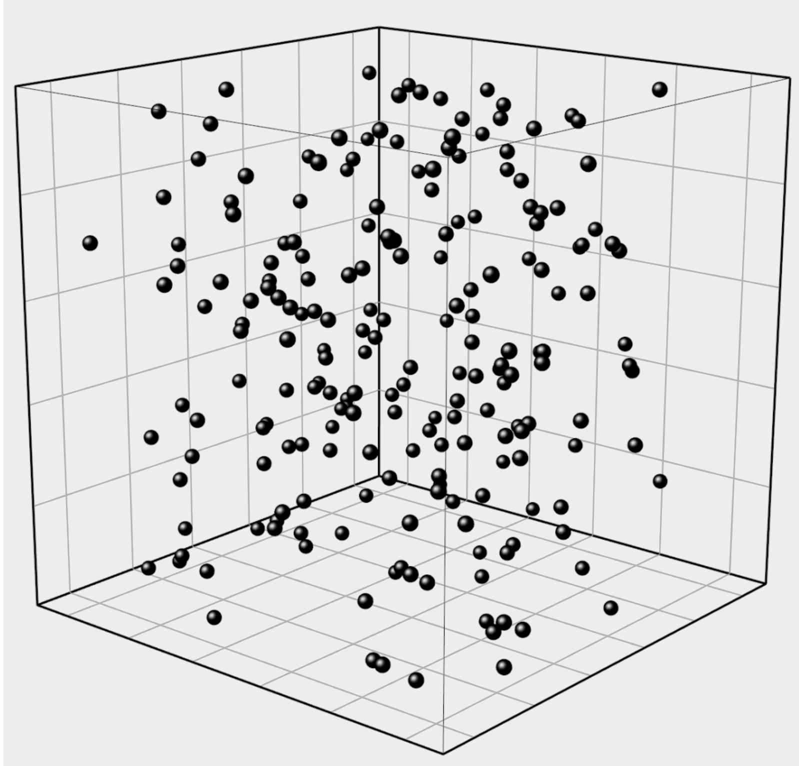

Figure 3a. Spatial Configuration of nanoparticles embedded in a crystal lattice.

b

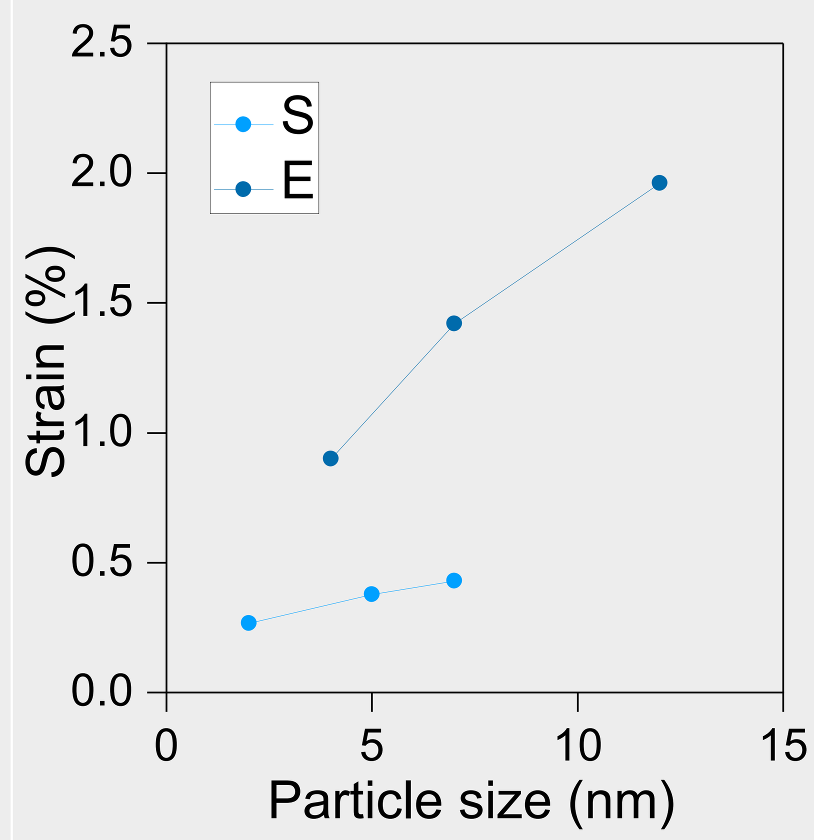

Figure 3b. Volumetric strain as a function of a particle size in an endo-particle system.

c

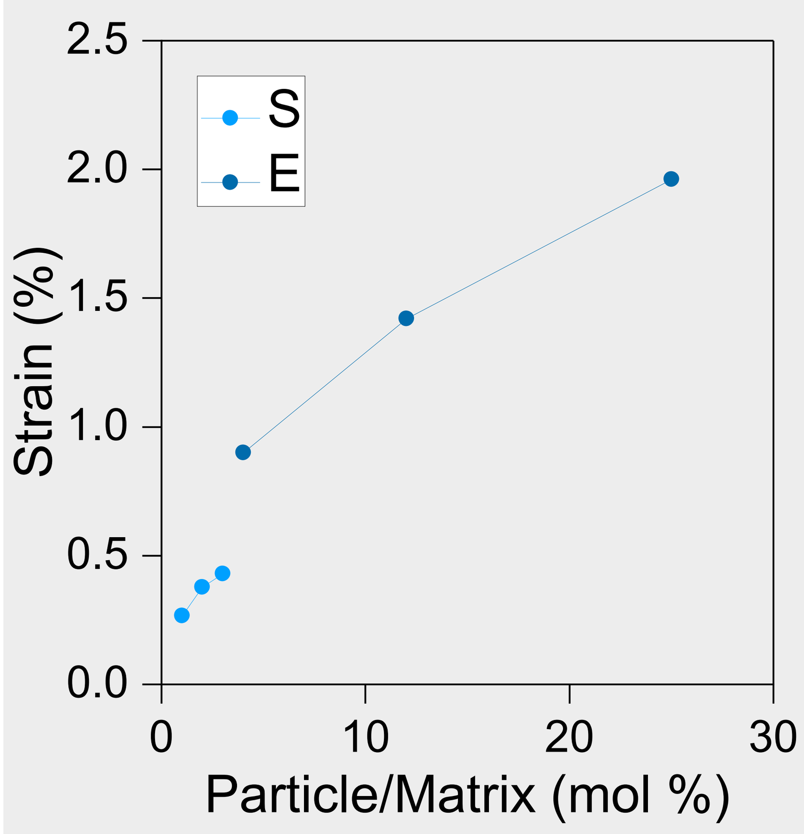

Figure 3c. Volumetric strain as a function of particle/matrix % loading.

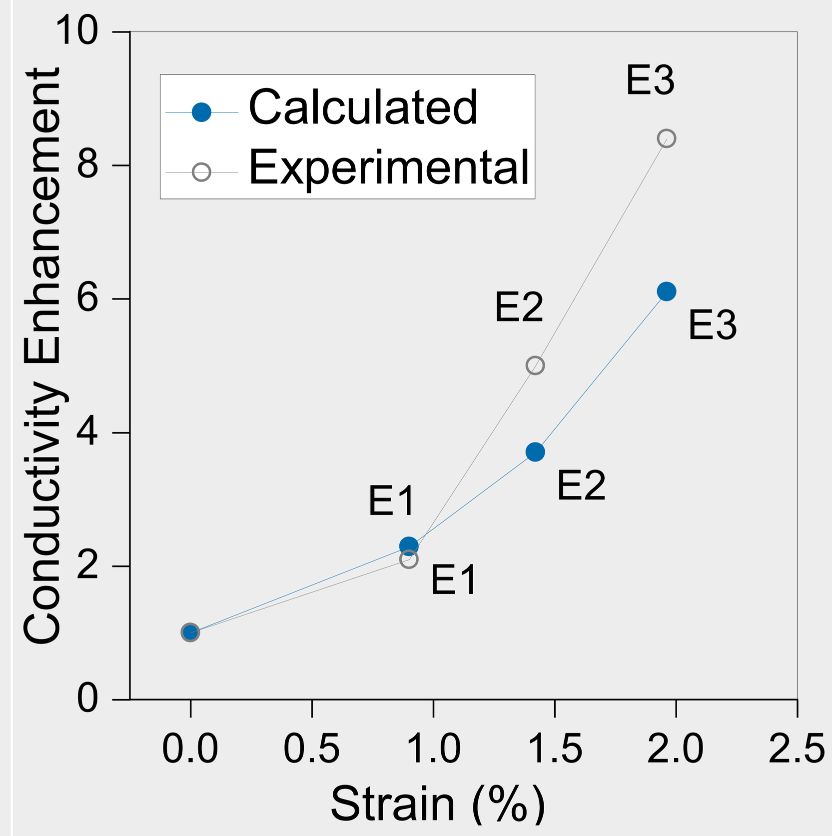

Figure 3d. Strain-conductivity model validation against experimental data for system E1-E3.

Discussion and Conclusion

System 'S' formed by sintering gold with PNCO at 873 K. System 'E' formed by the exsolution of nickel oxide from LTNO at 800 K. Expansive strain is proportional to the amount of embedded nanoparticles as seen in Figures 3b & 3c. For the E system in Figure 3d, the strain is approximately 1.05 –2.26% leading to an increased conductivity by a factor of 2.2 – 5.8.

- Experimental result explains the proposed strain-conductivity model (Figure 3d) thereby validating the methodology.

Future work

- Create strain in the novel electrolytes.
- Measurement of their ionic conductivities.

Acknowledgement

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