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Characterization of Lithium Lanthanum Zirconium Oxide (LLZO) for Structural and Phase Analysis in X-ray Diffraction for Li-ion Battery Applications

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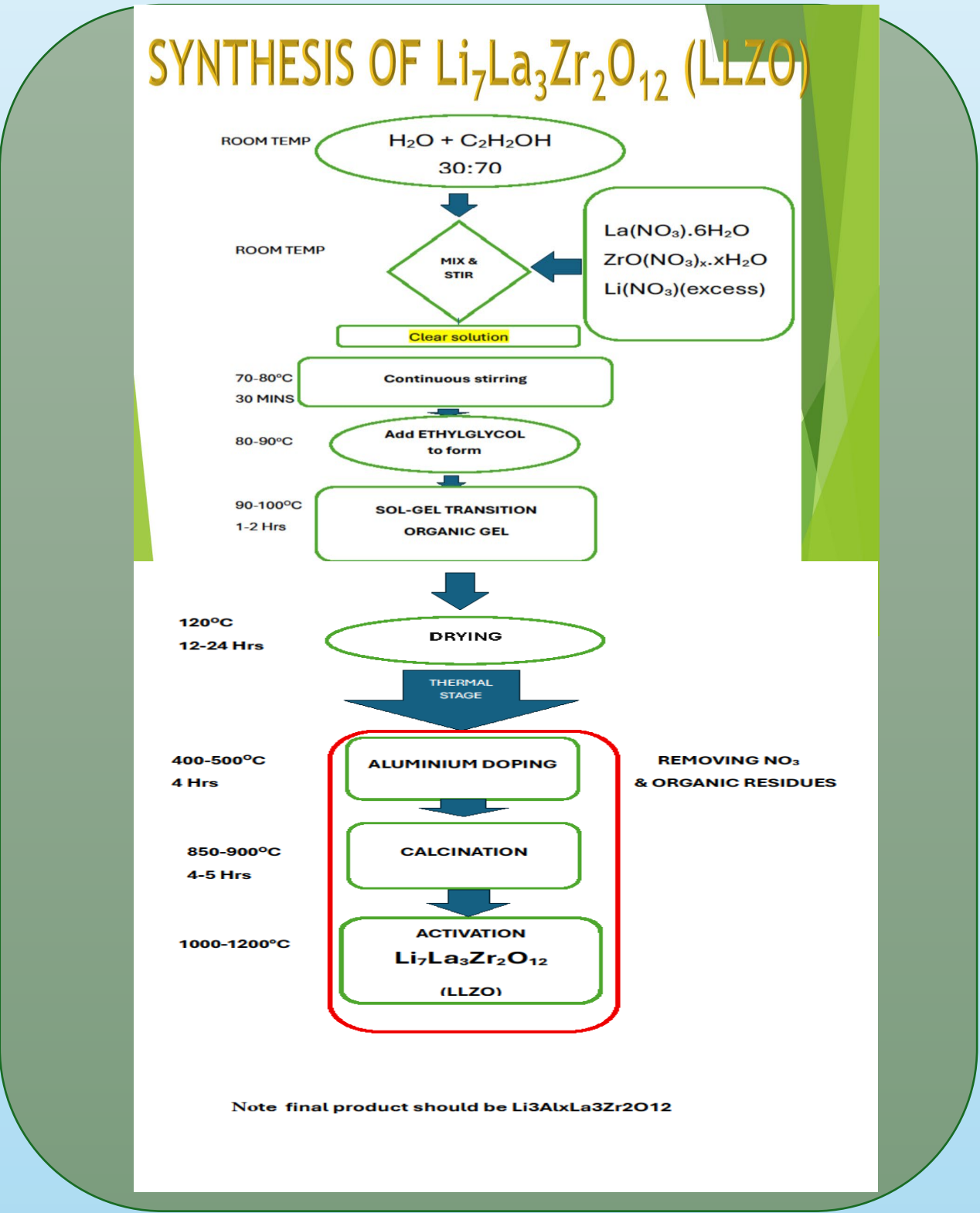
Introduction

AIM: Characterize Doped LLZO in XRD

OBJECTIVE: Compare LLZO to LLZO-Al

WHY?

To study SOLID STATE Electrolyte for Li-ion Batteries application



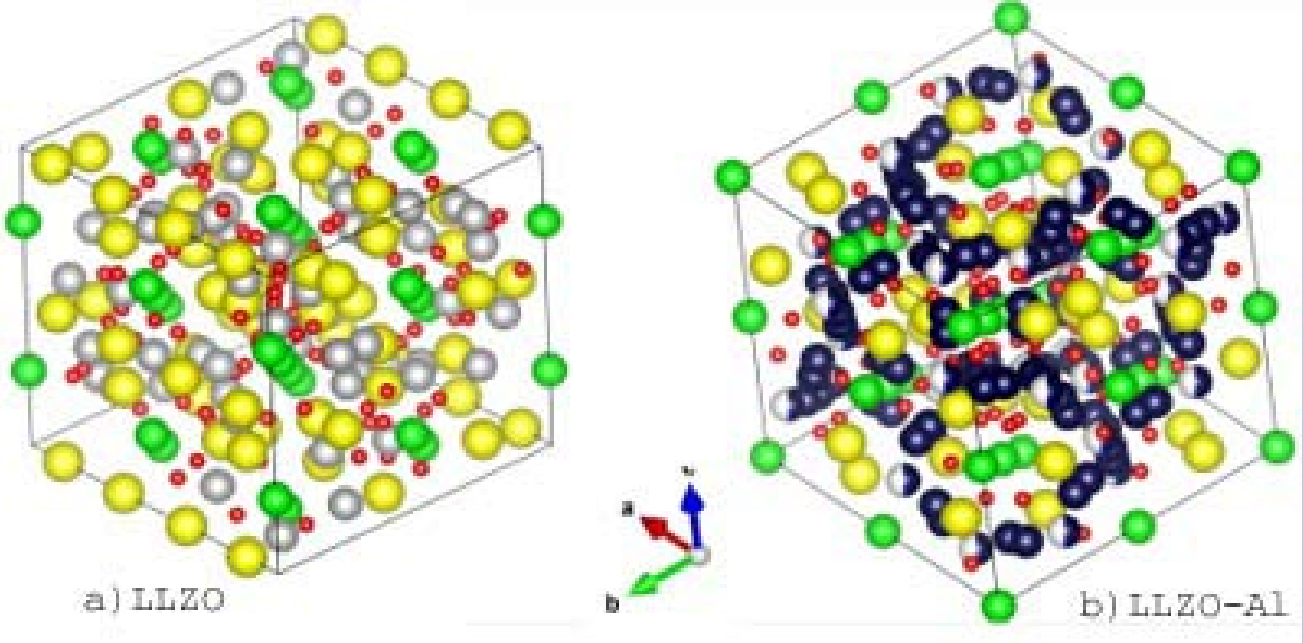
Conclusion

Al doping improves stabilization of LLZO, creating high ionic conductivity $\sim 10^{-3}$.

The Future:

Construction of a LLZO-Al solid-state Li-ion Battery.

Tetragonal & Cubic phase



1a) LLZO 1b) LLZO-Al [5]

LLZO-Al stabilization

UNIT CELL

UnDoped LZZO		
Site	Occupancy	
96 h	100% Li	full
24 d	45% Li	Partial
96 h	100% Li	full

Stable
Limited ionic
Conduction

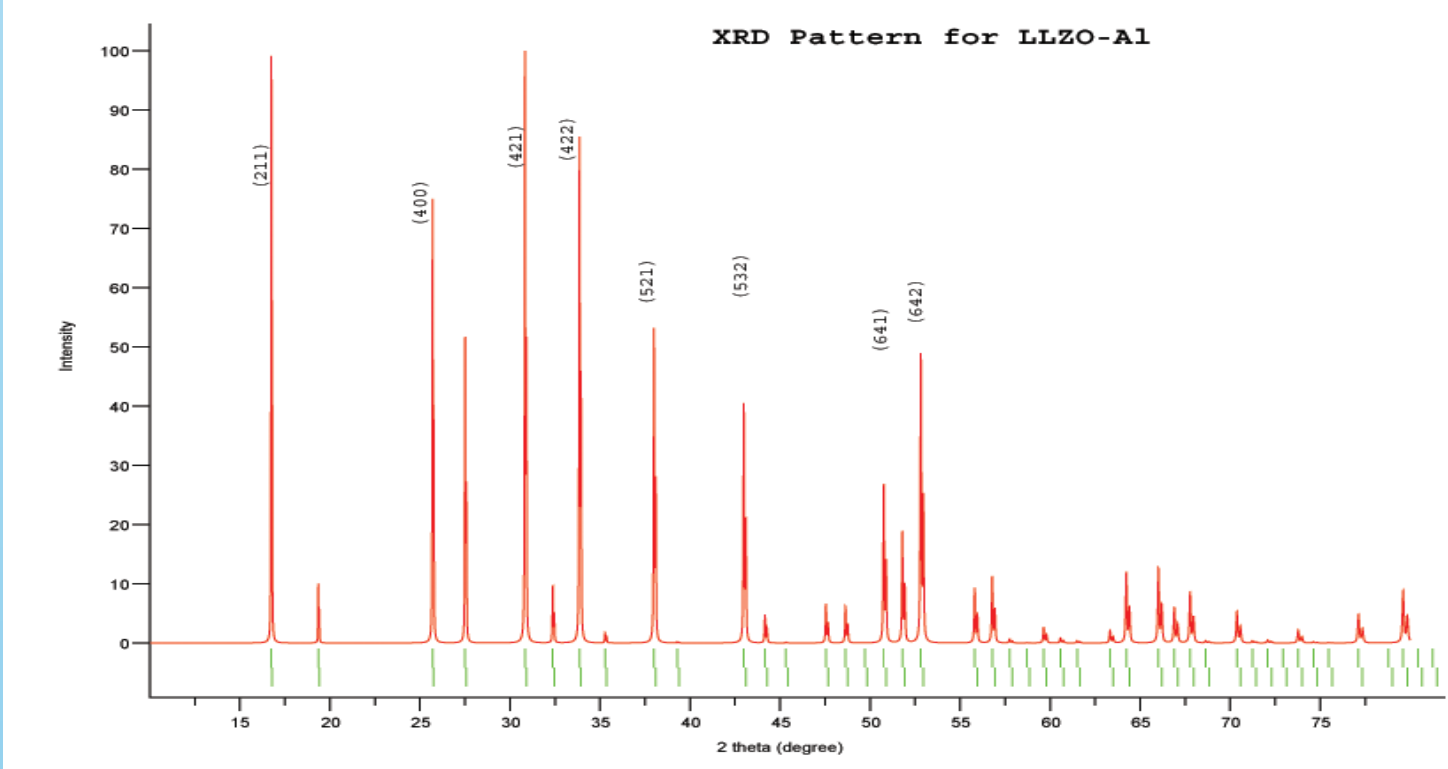
2a) Before doping

Doped LZZO		
site	Occupancy	
96 h	99% Li	Li vacancies
24 d	30% Li	Al ³⁺
96 h	99% Li	Li vacancies

Stable
Increased ionic
Conduction

Al³⁺ ejects 3 Li³⁺

2b) After Al-doping

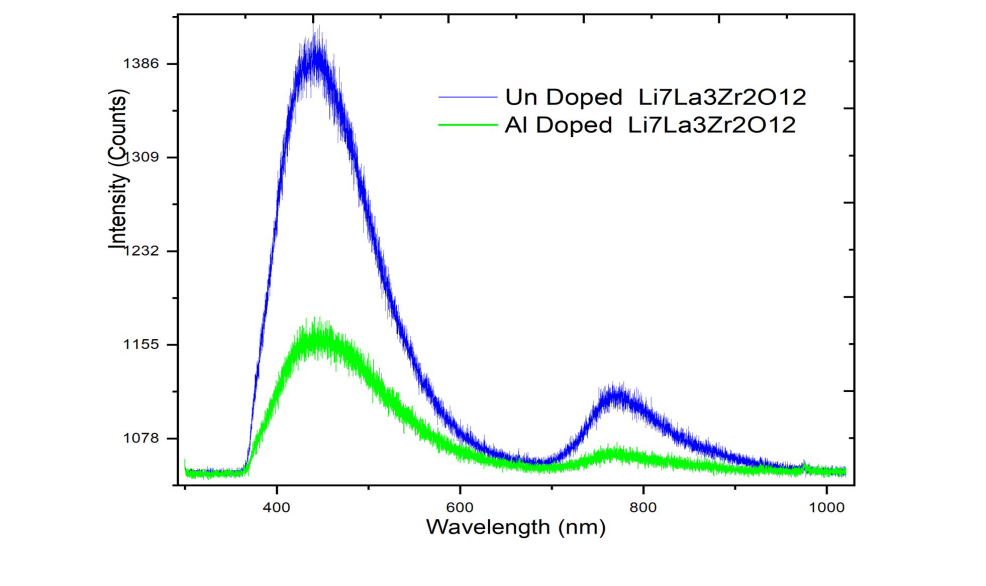


Graph 1: XRD intensity vs 2Θ (Range = 10°- 80°)

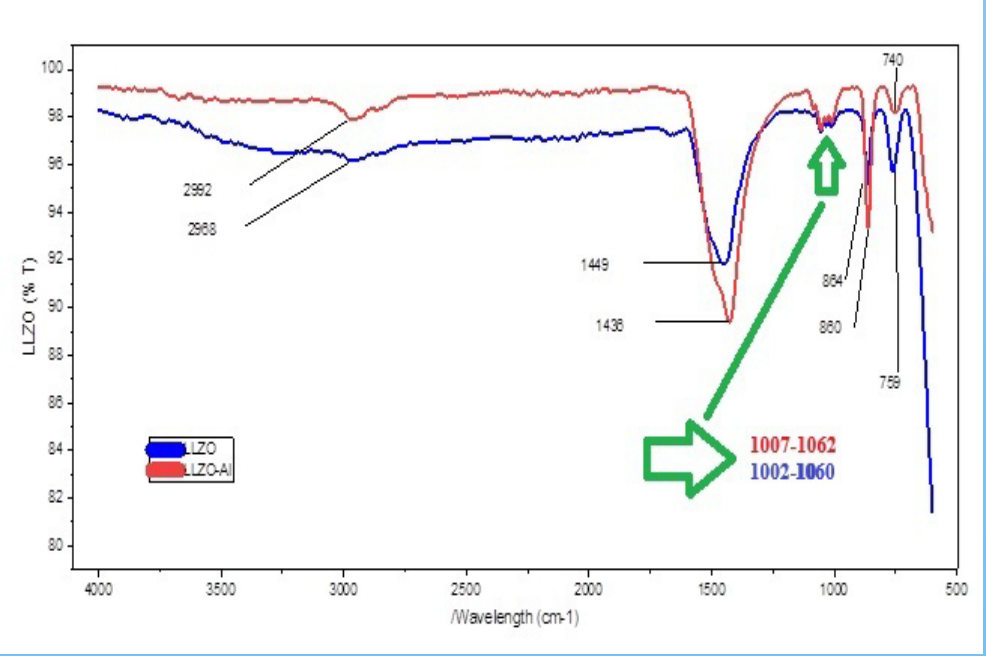
Rp = 9.1%	χ² = 2.3	
λ = 1.54 Å (Cu Kα)	2θ Range = 10°- 80°	
Space group = $1\bar{a} - 3d$	Phase LLZO-Al	(230)
a = 12.96 Å	b = 12.96 Å	c = 12.96 Å
Refinement: FullProf Suite version 2024		

Table 1: Preliminary Rietveld refinement [6]

Further RESULTS



Graph 2; Photoluminescence Intensity vs λ of LLZO & LLZO Al



Graph 3; FTIR spectrum of LLZO & LLZO-Al



Pic 1: Pre-Calcination Picture of synthesized LLZO

References

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7)etc

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