Application Note BATT1015

View on rigaku.com

BATT1015 - Local Structure Analysis of Li_3PS_4 Solid-State Electrolyte

Introduction

The crystalline structure of LPS is known to be related to its Li ion electric conductivity. However, as LPS exhibits low crystallinity near room temperature, applying traditional structural analysis methods, such as Rietveld analysis, proves difficult. Meanwhile, pair distribution function (PDF) analysis can analyze local atomic structures even with non- crystalline materials. For that reason, PDF analysis combined with the RMC (Reverse Monte Carlo) method was applied to investigate how LPS's disordered crystal structure relates to electric conductivity at varying temperatures. For details, please refer to the cited papers.

Crystal phase analysis

- **Analysis:** Solid-state electrolytes
- **Analysis method:** PDF analysis, RMC method
- **Use:** Improving ionic conductivity
- **Analyzed materials:** Li_3PS_4, LPS

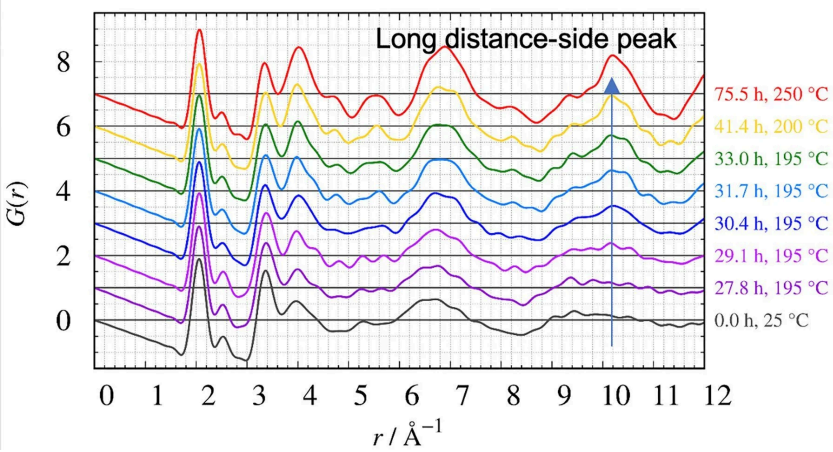

Figure 1: PDF analysis results obtained for each room temperature and retention time (y-axis: G(r); x-axis: interatomic distance)
When temperature rises, a long distance-side peak in interatomic distance is visible. As such, crystallization can be ascertained to be taking place.

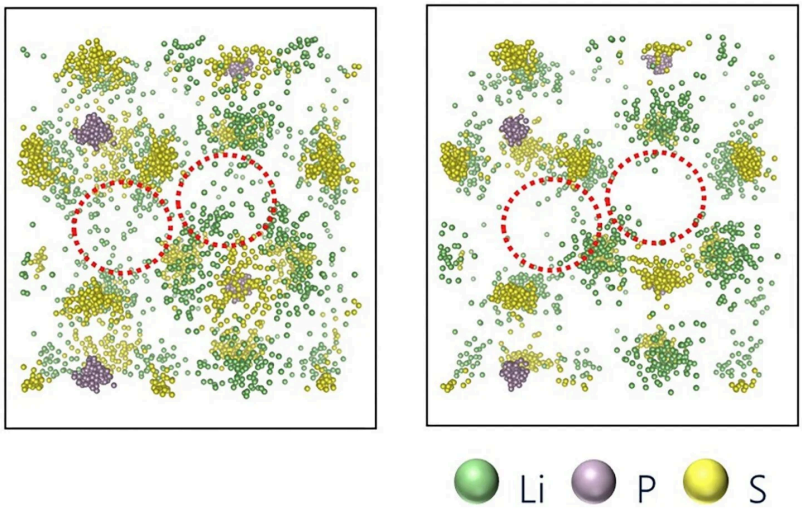

Figure 2: Crystalline structure at room temperature (298K) and 523K obtained through RMC method
It can be ascertained that the distribution of Li expands from the local structure circled above to a glass state.

Conclusion

By applying the RMC method using PDF analysis, which can be applied even to non-crystalline material, each crystal state can be analyzed.

Cited papers

M. Yoshimoto, T. Kimura, A. Sakuda, C. Hotehama, Y. Shiramata, A. Hayashi, K. Omote, *Solid State Ionics*, **401** (2023), 116361 (8pp).

Related products

SmartLab

Advanced state-of-the-art high-resolution XRD system powe
red by Guidance expert system software