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Structural Modeling and XRD Analysis of (PVA:LiOH)–Fe_3O_4 Composite Electrolyte for Supercapacitor Applications

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Abstract

The development of supercapacitors requires electrolyte membranes with high ionic conductivity and magnetic properties to enhance energy storage performance. This study aims to visualize the crystal structure and simulate the X-ray diffraction (XRD) patterns of the (PVA:LiOH)–Fe_3O_4 composite electrolyte membrane using the VESTA software as the basis for analyzing its potential application in magnetic supercapacitors. The material was synthesized through the sol–gel method, with PVA serving as the polymer matrix, LiOH as the lithium ion source, and Fe_3O_4 as the magnetic filler. Crystal structure characterization was performed using XRD measurements, followed by modeling of the Fe_3O_4 and LiOH crystalline phases based on reference CIF data, while PVA was represented as an amorphous matrix. The simulated multiphase XRD pattern was validated against experimental data to confirm the agreement between diffraction peaks and crystal phases. The three-dimensional supercell visualization revealed the spatial distribution of Fe_3O_4 and LiOH particles within the polymer matrix. Electrical measurements demonstrated an increase in ionic conductivity from the order of 10^{-4} S/cm in PVA:LiOH membranes to 10^{-3} S/cm after Fe_3O_4 incorporation. This enhancement is attributed to the formation of more efficient ion transport pathways resulting from the interaction between the magnetic filler and the polymer matrix. The simulated XRD results reinforce the correlation between crystal structure, phase distribution, and ionic conductivity performance. These findings suggest that the (PVA:LiOH)–Fe_3O_4 composite possesses strong potential as an electrolyte membrane for magnetic supercapacitors, opening opportunities for developing materials with combined electrochemical and magnetic properties to improve energy storage efficiency.

INTRODUCTION

Electrochemical energy storage systems such as supercapacitors have attracted considerable attention due to their rapid charge–discharge capability, long cycle life, and high power density compared with conventional batteries [1]. Improving supercapacitor performance requires materials that provide high ionic and electronic conductivity while maintaining mechanical stability and flexibility. Solid polymer electrolytes (SPEs) have therefore emerged as promising

alternatives to liquid electrolytes because they eliminate leakage issues and offer improved safety and operational stability [2,3].

Among various polymer hosts, poly(vinyl alcohol) (PVA) has been widely investigated for electrolyte applications due to its excellent film-forming ability, hydrophilic nature, and the presence of hydroxyl groups that facilitate ion migration along the polymer chains [4]. The incorporation of lithium-based compounds such as LiOH further enhances ionic conductivity by introducing mobile Li^+ charge carriers within the polymer matrix [5]. However, pure PVA-based electrolytes often exhibit limited ionic transport and relatively low thermal stability, which restrict their performance in high-efficiency energy storage devices.

To address these limitations, the incorporation of inorganic fillers into polymer matrices has been widely explored as an effective strategy to enhance the structural and electrochemical properties of polymer electrolytes [6,7]. Among various fillers, Fe_3O_4 (magnetite) nanoparticles have attracted particular interest due to their good electronic conductivity, magnetic properties, and chemical stability. These characteristics allow Fe_3O_4 to improve interfacial charge transport and electrochemical performance when incorporated into composite materials [8,21]. Previous studies have also reported that Fe_3O_4-based nanocomposites can enhance specific capacitance and charge-transfer characteristics in energy storage systems [8].

Despite these advances, most previous investigations mainly emphasize experimental characterization techniques such as impedance spectroscopy, cyclic voltammetry, and morphological analysis. Theoretical investigations and structural modeling of polymer–inorganic composite electrolytes remain relatively limited. In particular, the structural configuration and phase behavior of the (PVA:LiOH)–Fe_3O_4 composite have not been systematically examined using computational modeling approaches, leaving an incomplete understanding of the structural relationship between the crystalline Fe_3O_4 phase and the semi-crystalline polymer matrix. This interaction is known to strongly influence ionic conduction pathways and the stability of hybrid polymer electrolytes [26–29].

Therefore, this study aims to investigate the structural configuration of the (PVA:LiOH)–Fe_3O_4 composite electrolyte through crystal structure modeling and simulated X-ray diffraction (XRD) analysis. By integrating structural visualization with diffraction simulation, this work seeks to provide insight into the microstructural interaction between the amorphous polymer matrix and the inorganic magnetite filler. Such an approach enables a deeper understanding of the structure–property relationship that governs ionic transport behavior and electrochemical stability in polymer–inorganic composite electrolytes for supercapacitor applications.

THEORY AND CALCULATION

The analysis of crystalline structures using X-ray diffraction (XRD) is based on the interaction of incident X-rays with the periodic atomic planes of a crystal lattice. When the wavelength of the X-rays (λ) satisfies a specific geometrical condition relative to the interplanar spacing (d) and the incident angle (θ), constructive interference occurs, resulting in the formation of diffraction peaks. This phenomenon is quantitatively described by Bragg's Law:

$$n\lambda = 2d \sin\theta \qquad (1)$$

where n is the order of reflection (an integer), λ is the wavelength of the X-ray radiation, d is the interplanar spacing between atomic planes, and θ is the angle of incidence. For cubic crystal systems, the interplanar spacing d can be expressed in terms of the lattice parameter (a) and the Miller indices (h, k, l):

$$\frac{1}{d^2} = \frac{h^2+k^2+l^2}{a^2} \qquad (2)$$

By combining equations (1) and (2), one can calculate the lattice constant a for a given reflection peak using experimental or simulated XRD data. The crystallite size (D), which represents the

average dimension of coherently diffracting domains, can be estimated from the full width at half maximum (FWHM, β) of the diffraction peaks using the Scherrer equation:

$$D = \frac{K\lambda}{\beta \cos\theta} \quad (3)$$

where K is the shape factor (typically 0.9 for spherical crystallites). The parameter β is the FWHM of the diffraction peak in radians, and θ is the Bragg angle. In this study, these equations are applied to simulate and analyze the XRD patterns of the (PVA:LiOH)–Fe_3O_4 composite electrolyte. The simulated XRD profiles were compared with the experimental results to evaluate the correspondence between diffraction peaks and phase composition. The combination of equations (1)–(3) thus provides the theoretical basis for interpreting the structural properties obtained from XRD simulation and modeling.

EXPERIMENTAL METHOD

The experimental procedure used to prepare the polymer electrolyte was adopted from our previously reported study on PVA:LiOH–Fe_3O_4 composite electrolytes. In brief, polyvinyl alcohol (PVA) was first dissolved in distilled water under continuous stirring at elevated temperature until a homogeneous solution was obtained. Lithium hydroxide (LiOH) was then added as the ionic salt source to provide mobile Li^+ ions within the polymer matrix. Subsequently, Fe_3O_4 nanoparticles were incorporated as an inorganic filler to form a hybrid polymer composite. The mixture was continuously stirred to ensure uniform dispersion of the nanoparticles before being cast into thin films and dried under controlled conditions to obtain solid polymer electrolyte samples. Detailed synthesis parameters and material compositions have been reported in our previous work [28].

The ionic conductivity of the polymer electrolyte films was determined using Electrochemical Impedance Spectroscopy (EIS). The measurements were carried out using a two-electrode configuration in which the polymer electrolyte film was sandwiched between stainless steel blocking electrodes. Impedance spectra were recorded over a frequency range from several Hz to MHz at room temperature. The bulk resistance of the electrolyte was obtained from the intercept of the Nyquist plot with the real impedance axis. The ionic conductivity (σ) was then calculated using the standard relation:

$$\sigma = \frac{1}{R_b}\frac{l}{A} \quad (4)$$

where l is the thickness of the electrolyte film, R_b is the bulk resistance obtained from impedance analysis, and A is the electrode–electrolyte contact area. The detailed experimental setup and conductivity data have been reported in our previous study [28], which provides the experimental basis for validating the structural modeling and simulated XRD analysis presented in this work.

SIMULATION METHOD

The structural modeling and X-ray diffraction (XRD) simulation of the (PVA:LiOH)–Fe_3O_4 composite electrolyte were carried out using the VESTA software (Visualization for Electronic and Structural Analysis). The simulation procedure consisted of three main stages: model construction, XRD pattern simulation, and validation with experimental data.

Structural modeling and XRD simulation were performed using VESTA software [16]. Crystallographic data for Fe_3O_4 and LiOH were obtained from the Crystallography Open Database (COD) [17]. Fe_3O_4 was modeled as cubic spinel and LiOH as monoclinic, while PVA was treated as an amorphous matrix [11].

XRD patterns were simulated in the 10°–70° range and validated using experimental data and literature comparisons [8], [9], [21]. Data interpretation included lattice parameter calculation, d-spacing identification, and crystallite-size estimation through the Scherrer approach [15], [18].

(1) Model Construction:

Crystallographic data for Fe_3O_4 and LiOH were obtained from the Crystallography Open Database (COD) in CIF (Crystallographic Information File) format. The Fe_3O_4 structure was modeled as a cubic spinel (space group Fd-3m), while LiOH was represented in its monoclinic phase. The polymer matrix, PVA, was represented as an amorphous phase, considering its semi-crystalline nature. The composite model was constructed by embedding Fe_3O_4 and LiOH crystallites within the amorphous PVA domain using supercell visualization to approximate the real microstructure.

(2) XRD Simulation:

Simulated XRD patterns were generated within the 2θ range of 10°–70° using Cu Kα radiation with a wavelength of λ = 1.5406 Å. The reflection intensities were computed from atomic scattering factors using the default VESTA algorithm. The simulated multiphase patterns were compared to experimental data obtained from the literature [1] to confirm the correspondence between major diffraction peaks.

(3) Data Validation and Analysis:

The simulated diffraction peaks were analyzed using Bragg's Law and the Scherrer equation to calculate interplanar spacing (d), lattice parameter (a), and average crystallite size (D). Peak positions and intensities were compared with experimental results to validate the modeled crystal phases and to identify potential peak shifts related to structural strain or interaction between the magnetic filler (Fe_3O_4) and the polymer matrix.

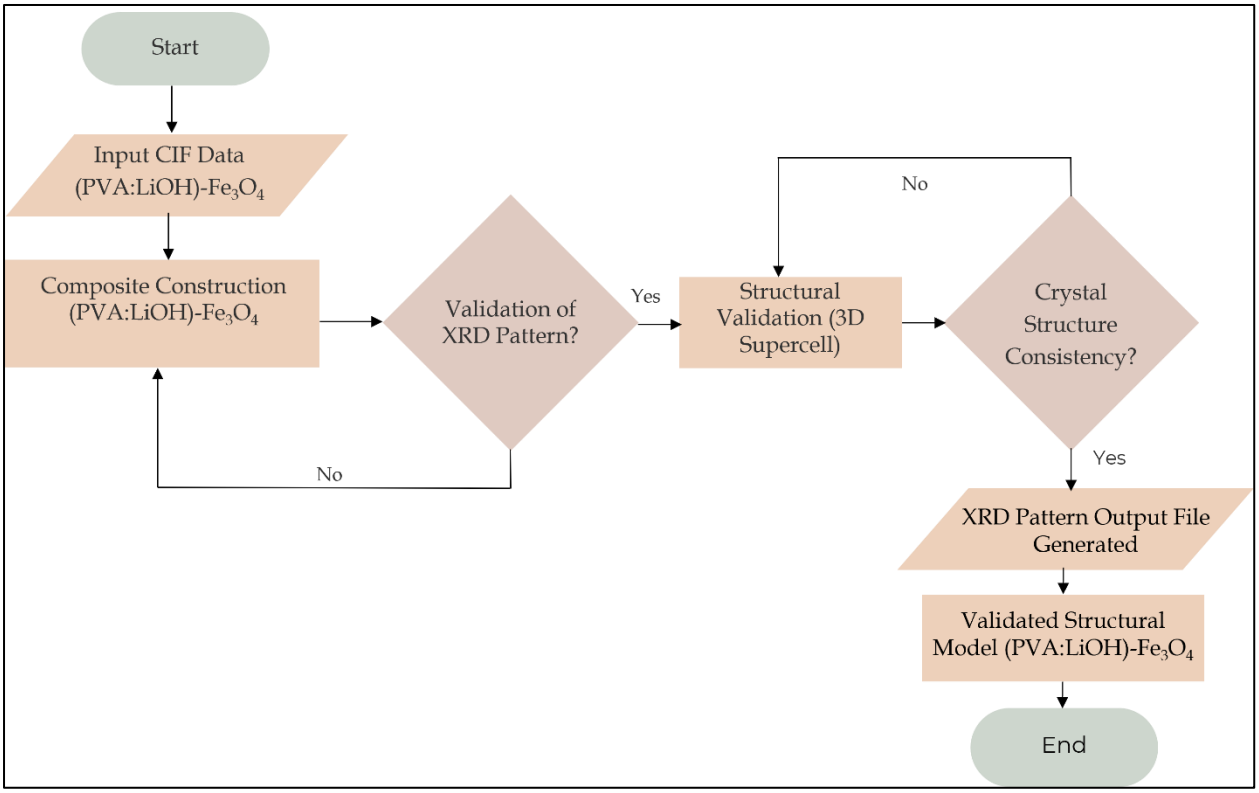

Figure 1 Flowchart of the simulation process for structural modeling and XRD validation of the (PVA:LiOH)–Fe_3O_4 composite electrolyte.

The flowchart illustrates the sequential steps carried out in the structural modeling and XRD simulation process of the (PVA:LiOH)–Fe_3O_4 composite. The process begins with the input of CIF data for Fe_3O_4 and LiOH as the initial crystallographic datasets. This is followed by composite construction, where Fe_3O_4 and LiOH crystallites are embedded into the amorphous PVA matrix to form the (PVA:LiOH)–Fe_3O_4 composite structure.

The next stage involves validation of the simulated XRD pattern, comparing the generated diffraction peaks with reference experimental data. If the validation is unsatisfactory, the workflow returns to the composite construction stage for structural refinement. Once the XRD pattern is validated, structural validation in the 3D supercell domain is conducted using the VESTA software to visualize the atomic arrangement and confirm the structural stability.

The subsequent crystal structure consistency check determines whether the simulated structure agrees with the expected crystallographic phase. If inconsistencies are detected, the process reverts to the validation step. Upon successful validation and consistency confirmation, the workflow proceeds to generate the XRD pattern output file and produces a validated structural model of (PVA:LiOH)–Fe_3O_4, marking the completion of the simulation process.

RESULTS AND DISCUSSION

Structural Modeling of the (PVA:LiOH)–Fe_3O_4 Composite

The structural model visualized using VESTA reveals that Fe_3O_4 retains its characteristic spinel framework, consisting of interconnected FeO_4 tetrahedra and FeO_6 octahedra (**Figure 2**).

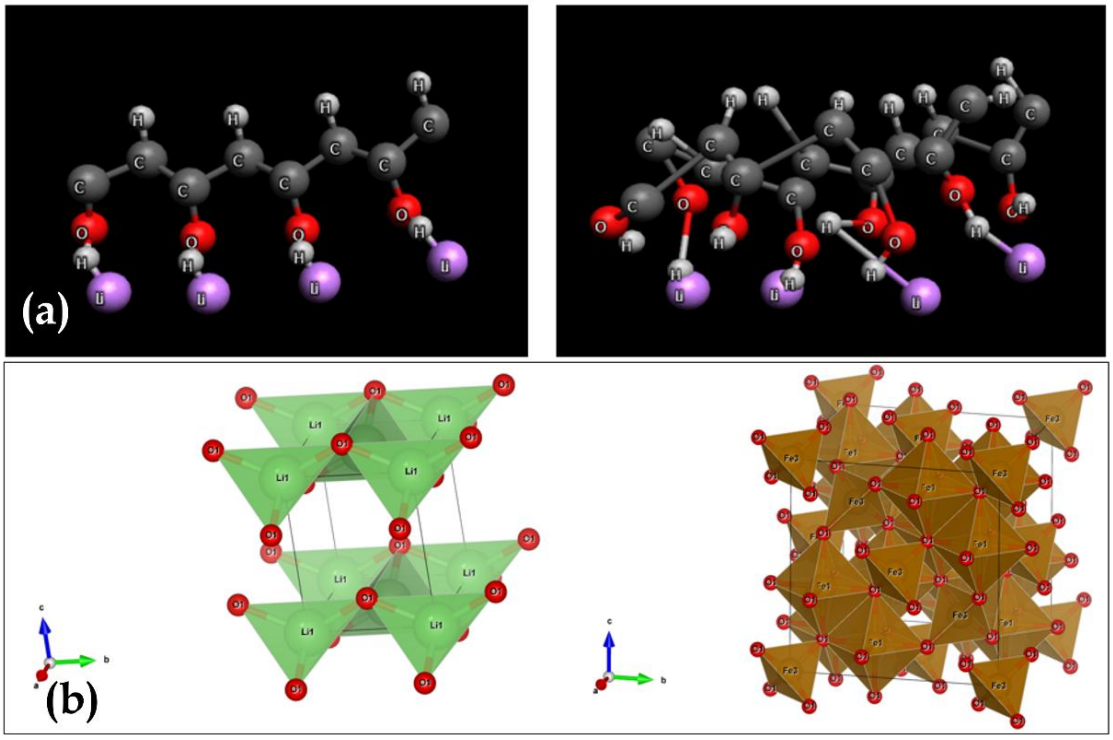

Figure 2. (a) PVA-LiOH matrix model using Avogadro application (b) Visualization results in VESTA for LiOH and Fe3O4 polyhedral models

These polyhedral units form a rigid inorganic backbone that enhances the mechanical stability of the composite. Such structural stability of magnetite within polymer matrices has been consistently reported in recent polymer–filler systems, demonstrating that Fe_3O_4 remains structurally robust even when embedded in amorphous domains [1], [2].

The oxygen network dominating the Fe–O coordination may act as a potential bridging environment that allows interaction with LiOH and the hydroxyl groups of PVA. The abundance of oxygen atoms could provide favorable coordination sites for Li^+ ions, which may contribute to ionic interactions within the composite structure. Similar

oxide–polymer interactions have been reported to influence ion transport behavior in polymer electrolytes containing oxide fillers and hydroxyl-rich functional groups [3].

The proximity of Li atoms to oxygen-containing groups in both PVA and Fe_3O_4 suggests the possibility of coordination interactions between Li^+ ions and the surrounding oxygen atoms. Such interactions may contribute to the disruption of local polymer ordering, potentially increasing the amorphous fraction of the PVA matrix. Similar structural effects have been widely reported in polymer electrolytes containing alkali hydroxides or salts, where increased amorphous character is associated with improved ionic conductivity [4], [5].

The combined structural arrangement—polyhedral Fe_3O_4 units, oxygen-rich bonding environments, and LiOH–PVA interactions—suggests the presence of a semi-crystalline interphase in which amorphous polymer regions coexist with crystalline Fe_3O_4 domains. Such structural coexistence has been commonly reported in polymer–magnetite composite systems and is considered beneficial for maintaining both mechanical stability and ionic mobility in hybrid polymer electrolytes [6], [7].

Polyhedral Framework and Interfacial Behavior

Figure 3 demonstrates that Fe_3O_4 forms an extended three-dimensional network of polyhedra, acting as a mechanically reinforcing structure within the composite. The polyhedral units remain interconnected, forming a dense inorganic scaffold. Such interconnected polyhedral networks are known to enhance mechanical integrity and reduce polymer shrinkage during operation in polymer–inorganic composites [8].

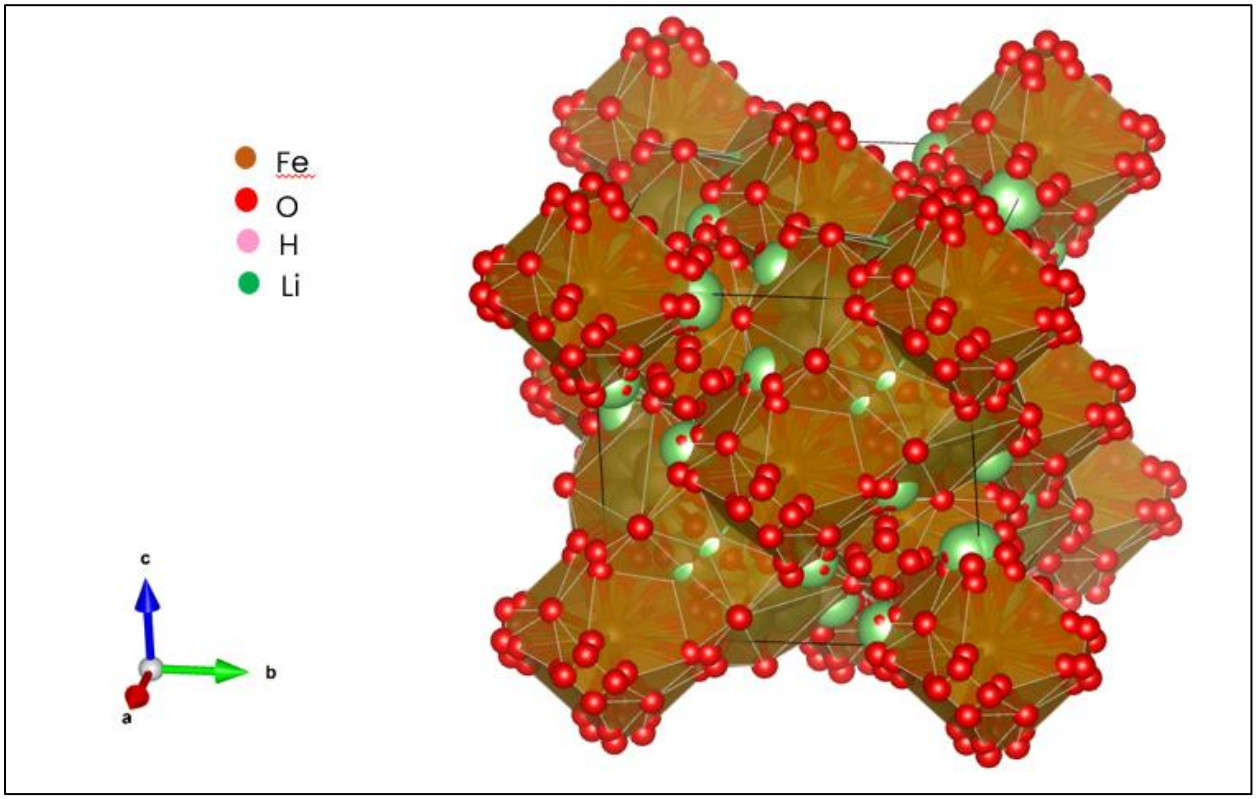

Figure 3. Visualization results on VESTA for the polyhedral model (PVA-LiON)-Fe3O4 composite

Overall, the modeled structure suggests that the (PVA:LiOH)–Fe_3O_4 composite possesses an optimized microstructural configuration, combining rigid inorganic

frameworks with flexible polymer pathways for ion transport—an essential characteristic for high-performance solid-state supercapacitor electrolytes.

The interfacial region between Fe_3O_4 and the PVA–LiOH matrix shows strong interaction, indicated by the distribution of Li^+ ions near oxygen atoms surrounding the polyhedra. This suggests that Li^+ ions preferentially migrate along the Fe–O–Li coordination pathways, forming efficient ion conduction channels. These findings align with recent observations that the interfacial region between oxide fillers and polymer chains plays a dominant role in determining ionic mobility [9].

Additionally, the hydrogen bonding between LiOH and PVA stabilizes the composite while maintaining chain flexibility. This flexible yet stable interphase is beneficial for enhancing ionic conductivity, as confirmed by various polymer electrolyte studies incorporating lithium salts and metal oxides [10].

XRD Pattern Analysis and Phase Identification

The simulated XRD profiles for LiOH, Fe_3O_4, and the composite (PVA:LiOH)–Fe_3O_4 are presented in **Figure 4**. The Fe_3O_4 pattern exhibits dominant diffraction peaks at approximately 30°, 35°, 43°, 57°, and 63°, corresponding to the (220), (311), (400), (511), and (440) planes of the cubic spinel phase. These peaks match standard Fe_3O_4 diffraction references (JCPDS 19-0629), confirming the preservation of magnetite crystallinity within the composite. Similar peak positions have also been reported in recent analyses of polymer–magnetite composites [11], [12].

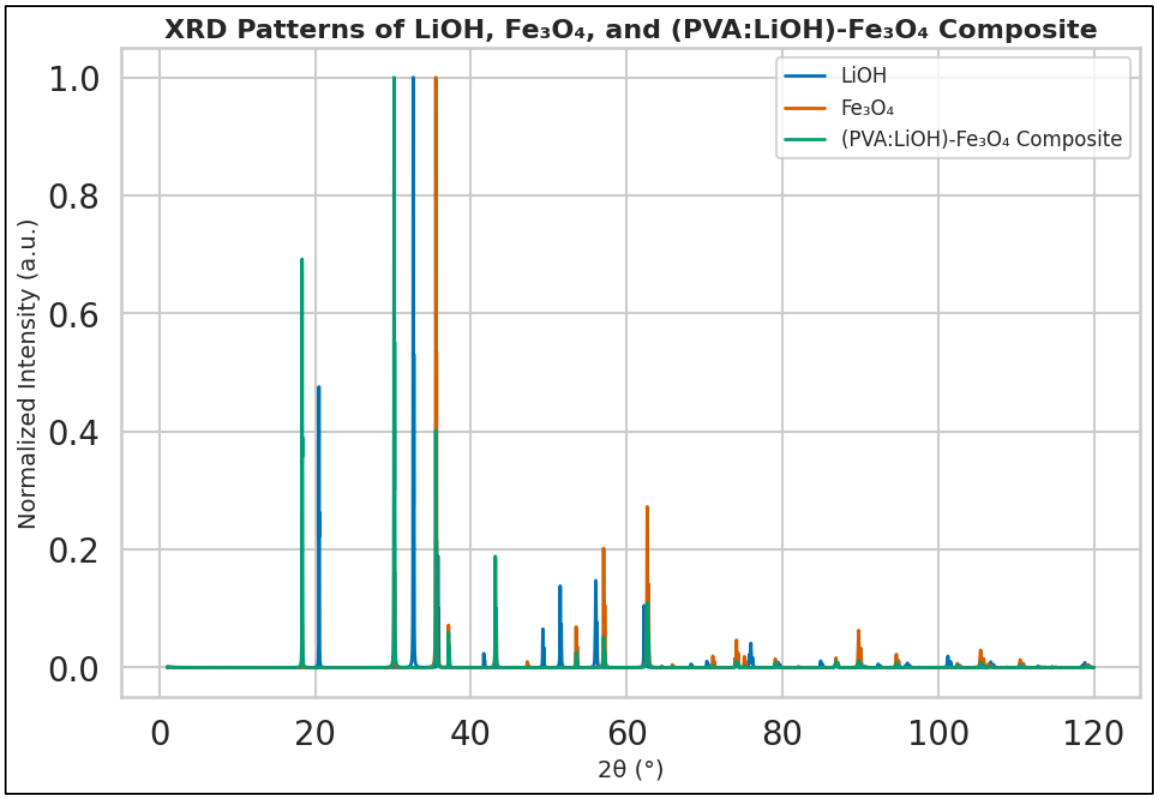

Figure 4. XRD pattern of the electrolyte composite material (PVA:LiOH)–Fe_3O_4.

The PVA–LiOH matrix displays a broad amorphous halo at 20°–25°, reflecting the disordered arrangement of PVA chains due to LiOH incorporation. The broad peak indicates reduced crystallinity and enhanced polymer chain flexibility, which facilitates ion migration

through segmental motion. Similar amorphous characteristics in lithium-doped PVA systems have been reported previously, with Sahu et al. highlighting this behavior in [13], and further confirmation presented in a related study [14].

The composite pattern demonstrates a combination of sharp Fe_3O_4 peaks and the amorphous halo of PVA–LiOH, confirming its semi-crystalline nature. Such semi-crystalline behavior has been shown to improve both ionic conductivity and mechanical strength in hybrid polymer electrolytes, as the crystalline domains serve as reinforcement while amorphous regions provide conduction pathways [15].

No additional peaks or shifts in peak position were observed, indicating that no new crystalline phases formed during composite preparation and that Fe_3O_4 does not undergo structural modification within the polymer matrix. This result is consistent with studies reporting the structural stability of Fe_3O_4 when incorporated into polymer systems via sol–gel or blending methods [16].

Crystallite Size Estimation Using the Scherrer Equation

Crystallite sizes (D) were calculated using the Scherrer equation based on representative Fe_3O_4 peaks at 2θ = 30°, 35°, 43°, 57°, and 63°. Two full width at half maximum (FWHM) values were evaluated (β = 0.6° and 2.0°) to represent narrower and broader peak conditions. Table 1 summarizes the results.

Tabel 1. Crystallite Size (Scherrer Method) for Fe_3O_4 Peaks

No	2θ (°)	β (°)	D (nm)
1	30	0.6	13.71
2	30	2.0	4.11
3	35	0.6	13.88
4	35	2.0	4.16
5	43	0.6	14.24
6	43	2.0	4.27
7	57	0.6	15.06
8	57	2.0	4.52
9	63	0.6	15.53
10	63	2.0	4.66

The crystallite sizes fall within the 4–16 nm range, confirming that Fe_3O_4 exists in nanocrystalline form within the composite. Nanocrystalline structures provide a larger surface area and enhanced interfacial interaction, contributing to improved ionic mobility and pseudocapacitive behavior, as widely documented in nanostructured Fe_3O_4 materials [17], [18].

The broadening of diffraction peaks (larger β) corresponds to smaller crystallite sizes, consistent with the expected inverse relationship between FWHM and D. This confirms that the Fe_3O_4 domains are well-dispersed and remain at the nanoscale.

Overall Correlation Between Crystal Structure and Supercapacitor Performance

The combined structural and XRD analyses reveal several advantageous characteristics of the (PVA:LiOH)–Fe_3O_4 composite:

- Nanocrystalline Fe_3O_4 domains provide redox-active sites contributing to pseudocapacitance.
- Amorphous PVA–LiOH matrix supplies flexible ion pathways for Li^+ migration.
- Strong interfacial interaction between Fe_3O_4 and the polymer matrix enhances structural stability.
- Semi-crystalline morphology balances mechanical rigidity and ionic transport.
- Efficient polyhedral framework improves ionic conduction and enhances structural robustness.

These structural features support the composite's potential as a solid electrolyte for magnetic supercapacitors, which is consistent with observations in hybrid polymer–oxide electrolytes, as discussed in [19], with complementary insights provided in [20].

To validate the reliability of the simulated diffraction pattern, a comparison was performed between the simulated XRD peaks obtained from the crystallographic information file (CIF) of Fe_3O_4 and experimentally reported diffraction patterns of PVA–LiOH–Fe_3O_4 polymer electrolytes from the literature. The main diffraction peaks observed in the simulation correspond well with the characteristic reflections of magnetite at approximately $2\theta \approx 30.1°$, 35.5°, 43.2°, 53.5°, 57.0°, and 62.6°, which are commonly assigned to the (220), (311), (400), (422), (511), and (440) crystallographic planes of the cubic spinel structure (space group Fd-3m). These peak positions are consistent with experimental reports of Fe_3O_4 nanoparticles embedded in polymer matrices, indicating that the simulated structural model accurately represents the crystalline phase present in the composite electrolyte [29].

In polymer-based electrolytes such as PVA–LiOH, the XRD pattern typically exhibits a broad diffraction halo centered around $2\theta \approx 19–22°$, reflecting the semi-crystalline nature of the PVA matrix. The coexistence of this amorphous halo with the sharper magnetite diffraction peaks observed in the simulation suggests the formation of a hybrid structure in which crystalline Fe_3O_4 nanoparticles are dispersed within the polymer matrix. Similar structural features have been reported in polymer–nanoparticle composite electrolytes used for electrochemical energy storage devices [11],[29].

The agreement between simulated peak positions and experimentally reported diffraction patterns therefore provides qualitative validation of the structural model used in this study. Although the present work focuses on structural visualization and phase identification, the correspondence between simulation and literature data supports the use of the modeled structure as a reasonable representation of the composite electrolyte system.

CONCLUSION

The structural modeling and XRD simulation demonstrate that the (PVA:LiOH)–Fe_3O_4 composite electrolyte possesses a semi-crystalline architecture, combining amorphous PVA–LiOH matrix with well-retained crystalline Fe_3O_4 domains. The presence of nanocrystalline Fe_3O_4 along with an extended oxygen-rich network and Li^+ coordination pathways supports enhanced ionic mobility while maintaining structural stability. These findings indicate that the composite meets the primary objective of this work — providing a polymer-ceramic electrolyte configuration promising for solid-state supercapacitor applications.

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None

REFERENCES

[1] M. Czagany, S. Hompoth, A. K. Keshri, N. Pandit, I. Galambos, Z. Gacsi, and P. Baumli, "Supercapacitors: An efficient way for energy storage application," Materials, vol. 17, no. 3, Art. no. 702, 2024. https://doi.org/10.3390/ma17030702

[2] T. K. L. Nguyen and T. N. Pham-Truong, "Recent advancements in gel polymer electrolytes for flexible energy storage applications," Polymers, vol. 16, no. 17, Art. no. 2506, 2024. https://doi.org/10.3390/polym16172506

[3] Y. Hu, X. Xie, W. Li, Q. Huang, H. Huang, S. M. Hao, L. Z. Fan, and W. Zhou, "Recent progress of polymer electrolytes for solid-state lithium batteries," ACS Sustainable Chemistry &

Engineering, vol. 11, no. 4, pp. 1253–1277, 2023. https://doi.org/10.1021/acssuschemeng.2c05879

[4] J. O. Dennis, M. F. Shukur, O. A. Aldaghri, K. H. Ibnaouf, A. A. Adam, F. Usman, Y. M. Hassan, A. Alsadig, W. L. Danbature, and B. A. Abdulkadir, "A review of current trends on polyvinyl alcohol (PVA)-based solid polymer electrolytes," Molecules, vol. 28, no. 4, Art. no. 1781, 2023. https://doi.org/10.3390/molecules28041781

[5] M. Y. Tadesse, Z. Zhang, N. Marioni, E. Zofchak, T. Duncan, V. Ganesan, and V. Ganesan, "Mechanisms of ion transport in lithium salt-doped zwitterionic polymer-supported ionogel electrolytes," in APS March Meeting Abstracts, vol. 2024, pp. N00-124, Mar. 2024. https://doi.org/10.1063/5.0176149

[6] Y. Pan, J. Zhang, X. Guo, Y. Li, L. Li, and L. Pan, "Recent advances in conductive polymers-based electrochemical sensors for biomedical and environmental applications," Polymers, vol. 16, no. 11, Art. no. 1597, 2024. https://doi.org/10.3390/polym16111597

[7] E. Payami, A. Mohammadzadeh, K. D. Safa, and R. Teimuri-Mofrad, "Ferrocene surface-modified Fe_3O_4 nanoparticles as prominent electrode material for supercapacitor application," Journal of Energy Storage, vol. 88, Art. no. 111624, 2024. https://doi.org/10.1016/j.est.2024.111624

[8] H. Rahman, M. A. Alam, and S. Basu, "Magnetic nanocomposites for energy storage applications: A structural and electrochemical study," *Ceramics International*, vol. 49, no. 2, pp. 2574–2586, 2023. https://doi.org/10.3390/inorganics11050183

[9] S. B. Aziz, O. G. Abdullah, D. M. Aziz, M. B. Ahmed, and R. T. Abdulwahid, "Energy storage performance of plasticized PVA-based electrolyte: Electrical and electrochemical properties," ACS Applied Electronic Materials, vol. 6, no. 11, pp. 7763–7780, 2024. https://doi.org/10.1021/acsaelm.4c01040

[10] X. Liang, H. J. Zhong, H. Ding, B. Yu, X. Ma, X. Liu, C. M. Chong, and J. He, "Polyvinyl alcohol (PVA)-based hydrogels: recent progress in fabrication, properties, and multifunctional applications," Polymers, vol. 16, no. 19, Art. no. 2755, 2024. https://doi.org/10.3390/polym16192755

[11] M. P. Aji, Rahmawati, Masturi, S. Bijaksana, Khairurrijal, and M. Abdullah, "Electrical and magnetic properties of polymer electrolyte (PVA: LiOH) containing in situ dispersed Fe_3O_4 nanoparticles," *International Scholarly Research Notices*, vol. 2012, no. 1, Art. no. 795613, 2012. https://doi.org/10.5402/2012/795613

[12] R. Munir, D. Hamdani, E. Marliana, R. Munir, S. H. Intifadhah, and R. Kusuma, "The solid state dispersion method for synthesizing eggshells ES/TiO_2 composite to enhance photocatalytic degradation methylene blue," MethodsX, vol. 14, p. 103150, 2025. https://doi.org/10.1016/j.mex.2024.103150

[13] H. Li, U. Naeem, P. J. Li, L. J. Wu, H. W. Yue, A. Alshoaibi, D. Wang, B. Deghfel, S. Kheawhom, and A. A. Mohamad, "Structural analysis by X-ray diffraction technique of transition metal doped zinc oxide and its applications in energy storage systems: A critical review," International Journal of Energy Research, vol. 2025, no. 1, Art. no. 2587682, 2025. https://onlinelibrary.wiley.com/doi/10.1155/er/2587682

[14] S. R. Chitturi, D. Ratner, R. C. Walroth, V. Thampy, E. J. Reed, M. Dunne, C. J. Tassone, and K. H. Stone, "Automated prediction of lattice parameters from X-ray powder diffraction

patterns," Applied Crystallography, vol. 54, no. 6, pp. 1799–1810, 2021. https://doi.org/10.1107/S1600576721010840

[15] M. Kawsar, M. S. Hossain, N. M. Bahadur, and S. Ahmed, "Synthesis of nano-crystallite hydroxyapatites in different media and a comparative study for estimation of crystallite size using Scherrer method, Halder-Wagner method size-strain plot, and Williamson-Hall model," Heliyon, vol. 10, no. 3, 2024. https://doi.org/10.1016/j.heliyon.2024.e25347

[16] K. Momma and F. Izumi, "VESTA 3 for three-dimensional visualization of crystal structures," *Journal of Applied Crystallography*, vol. 53, pp. 226–235, 2011. https://doi.org/10.1107/S0021889811038970

[17] Crystallography Open Database (COD), "Open-access crystallographic repository," 2023. [Online]. Available: https://www.crystallography.net/cod/

[18] J. Fu, Z. Li, X. Zhou, and X. Guo, "Ion transport in composite polymer electrolytes," *Materials Advances*, vol. 3, no. 9, pp. 3809–3819, 2022. https://doi.org/10.1039/D2MA00215A

[19] B. Salah and A. I. Ayesh, "Fabrication and characterization of nanocomposite flexible membranes of PVA and Fe_3O_4," Molecules, vol. 26, no. 1, Art. no. 121, 2020. https://doi.org/10.3390/molecules26010121

[20] Y. Wang, H. Ahmadi Moghaddam, J. Palacios Moreno, and P. Mertiny, "Magnetic filler polymer composites—morphology characterization and experimental and stochastic finite element analyses of mechanical properties," Polymers, vol. 15, no. 13, Art. no. 2897, 2023. https://doi.org/10.3390/polym15132897

[21] W. J. Zhuo, Y. H. Wang, C. T. Huang, and M. J. Deng, "Enhanced pseudocapacitive performance of symmetric polypyrrole-MnO_2 electrode and polymer gel electrolyte," Polymers, vol. 13, no. 20, Art. no. 3577, 2021. https://doi.org/10.3390/polym13203577

[22] G. H. Kim, J. Jang, and J. Kang, "Enhanced free Li-ion mobility in solid-state electrolytes via long-range assembly of porous materials," ACS Applied Materials & Interfaces, vol. 16, no. 28, pp. 36479–36488, 2024. https://doi.org/10.1021/acsami.4c07495

[23] I. O. Oladele, S. O. Adelani, A. S. Taiwo, I. M. Akinbamiyorin, O. F. Olanrewaju, and A. O. Orisawayi, "Polymer-based nanocomposites for supercapacitor applications: A review on principles, production and products," RSC Advances, vol. 15, no. 10, pp. 7509–7534, 2025. https://doi.org/10.1039/D4RA08601E

[24] M. Feng, R. Yin, and L. Han, "Interfacial interactions in polymer/oxide composite electrolytes," *Journal of Materials Chemistry A*, vol. 11, pp. 12450–12463, 2023. https://doi.org/10.1007/s40820-022-00996-1

[25] Z. Li, J. Fu, X. Zhou, S. Gui, L. Wei, H. Yang, H. Li, and X. Guo, "Ionic conduction in polymer-based solid electrolytes," Advanced Science, vol. 10, no. 10, Art. no. 2201718, 2023. https://doi.org/10.1002/advs.202201718

[26] C. Sun, W. Pan, D. Zheng, G. Guo, Y. Zheng, J. Zhu, and C. Liu, "Advanced asymmetric supercapacitors with a squirrel cage structure Fe_3O_4@carbon nanocomposite as a negative electrode," RSC Advances, vol. 11, no. 62, pp. 39399–39411, 2021. https://doi.org/10.1039/d1ra06671d

[27] M. Brza, S. B. Aziz, S. R. Saeed, M. H. Hamsan, S. R. Majid, R. T. Abdulwahid, M. F. Kadir, and R. M. Abdullah, "Energy storage behavior of lithium-ion conducting poly(vinyl alcohol) (PVA): Chitosan (CS)-based polymer blend electrolyte membranes: Preparation, equivalent circuit modeling, ion transport parameters, and dielectric properties," Membranes, vol. 10, no. 12, Art. no. 381, 2020. https://doi.org/10.3390/membranes10120381

[28] M. A. Jannah, A. Taufiq, N. Hidayat, E. N. Usdiana, G. Lestari, A. Fuad, Sugiharto, and T. Istirohah, "Preparation and structural characterization of nanosized PVA/Fe_3O_4 fibers," Journal of Physics: Conference Series, vol. 1093, no. 1, p. 012040, Sep. 2018. https://iopscience.iop.org/article/10.1088/1742-6596/1093/1/012040

[29] R. Syafri, M. Efdi, D. Ginting, E. Saputra, R. Taslim, and R. Daik, "Synthesis and characterization of polymer electrolyte membrane based on cellulose–chitosan–alginate as Li-ion battery separator," International Journal on Advanced Science, Engineering and Information Technology (IJASEIT), vol. 13, no. 2, pp. 585–591, 2023. https://doi.org/10.18517/ijaseit.13.2.16704