

Research Highlight

How electrode microstructure evolves in Li ions battery

Weibin Yan¹, Yu Li^{2,*}

¹Laboratory of Inorganic Materials Chemistry (CMI), University of Namur, 61 Rue de Bruxelles, Namur 5000, Belgium.

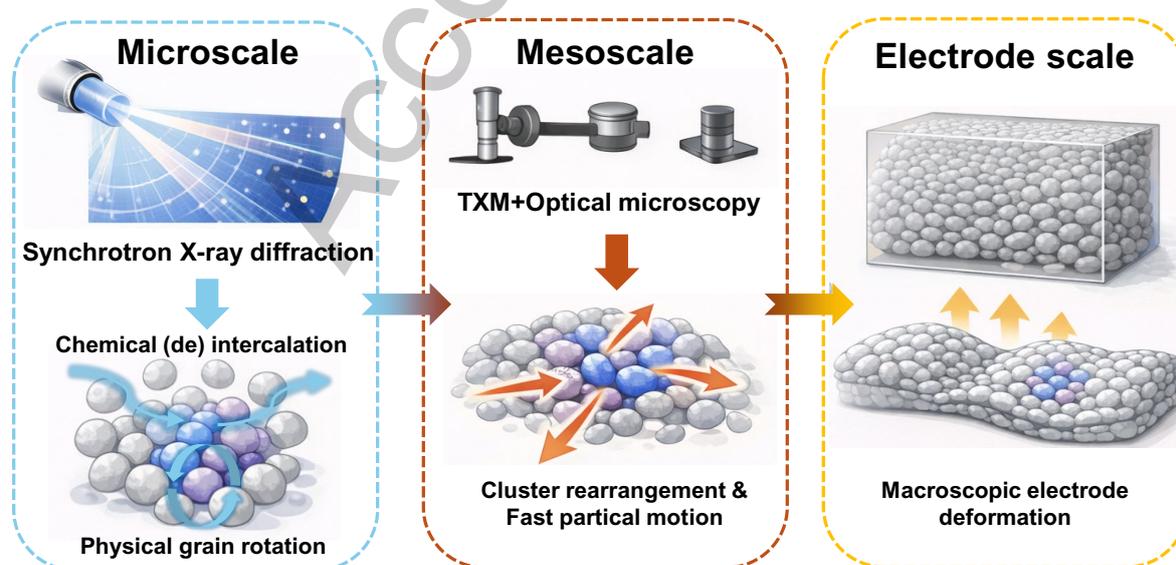
²Laboratory of Living Materials at the State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, Wuhan 430070, Hubei, China.

***Correspondence to:** Yu Li, Laboratory of Living Materials at the State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, Wuhan 430070, Hubei, China. E-mail: yu.li@whut.edu.cn

How to cite this article: Yan W, Li Y. How electrode microstructure evolves in Li ions battery. *Chem Synth* 2026;6:[Accept]. <http://dx.doi.org/10.20517/cs.2026.05>

Received: 13 January 2026 | **Revised:** 27 February 2026 | **Accepted:** 16 March 2026

Graphical Abstract:



Keywords: Strain cascade, asynchronous electrochemistry, intercalation cathodes, operando multimodal microscopy

Intercalation-based electrodes form the foundation of modern lithium-ion battery technologies, yet their long-term reliability is fundamentally constrained by chemomechanical degradation^[1]. Electrochemical cycling induces heterogeneous structural changes within electrodes, leading to cracking, swelling, and irreversible deformation across multiple length scales^[2]. Although heterogeneous structural responses under static conditions have been extensively characterized, revealing significant inter- and intra-particle heterogeneity^[3, 4], how these particle-scale electrochemical differences collectively evolve into electrode-scale strain and macroscopic deformation remains a critical unresolved issue^[5]. Writing in *Science*, Yijin Liu, Juner Zhu, and colleagues provide compelling real-time evidence that electrode deformation emerges from a cascading chemomechanical process driven by asynchronous electrochemical evolution across particles and grains, thereby redefining the origin of mechanical fatigue in intercalation cathodes^[6].

Using multimodal operando microscopy methods, the authors directly visualize how heterogeneous state-of-charge (SOC) evolution generates internal stress that progressively reorganize electrode microstructures. In a free-standing layered NMC cathode, operando spectro-transmission x-ray microscopy (TXM) reveals that neighboring particles undergo coordinated translational and rotational motion during slow charging, gradually moving into physical contact [Figure 1A]. Crucially, despite concurrent delithiation, adjacent particles retain distinct SOC levels for extended periods, demonstrating persistent electrochemical asynchronicity at the particle level. These SOC disparities diminish only after physical contact is established, consistent with microscale charge redistribution and redox coupling [Figure 1B]. These observations establish that electrode strain is not a passive consequence of uniform lattice expansion, but an emergent response to asynchronous electrochemical evolution among interacting particles.

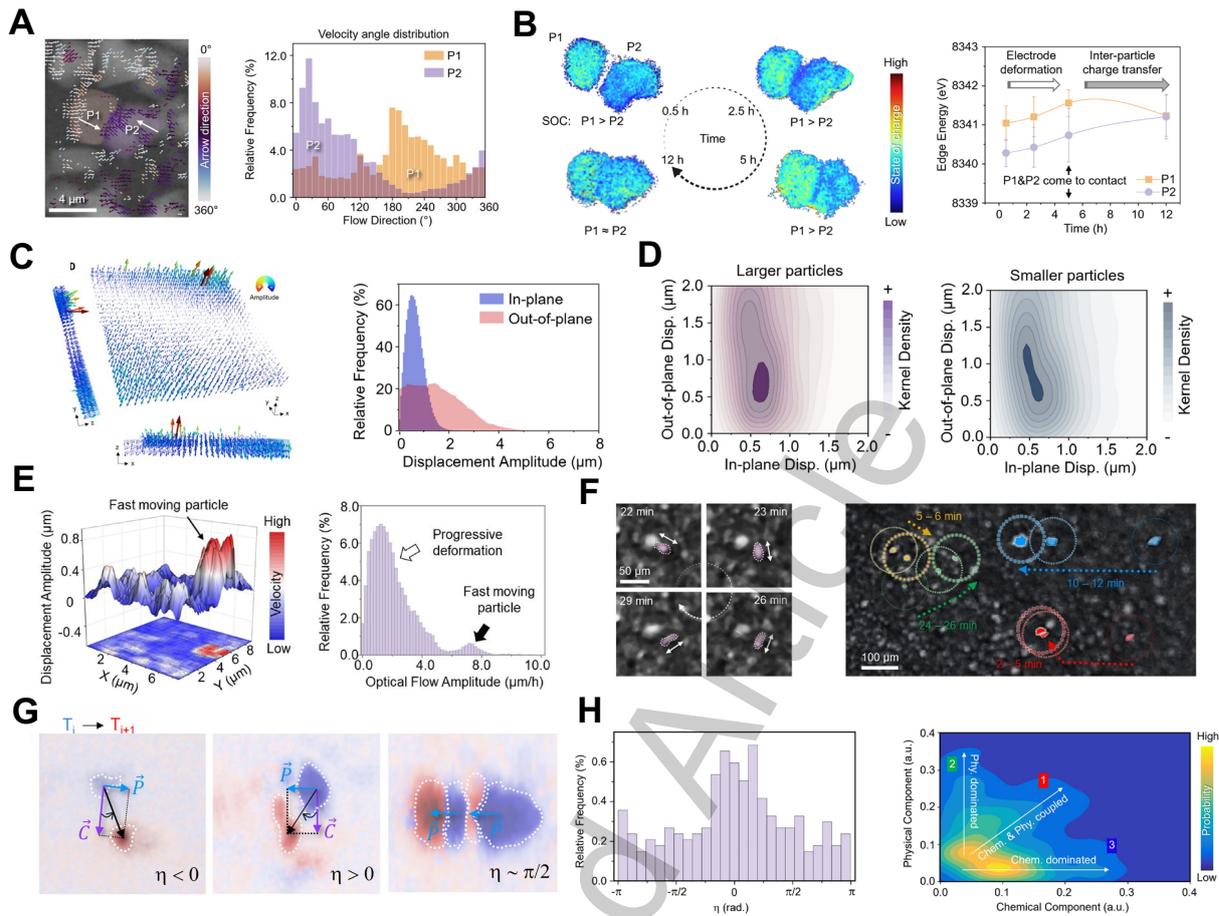


Figure 1. (A) Optical flow analysis of the particle motion and probability distribution of the local velocity angles in P1 and P2 particles; (B) TXM SOC mapping using Ni K-edge energy, and the evolution of mean value and standard deviation of P1 and P2 particles' Ni K-edge energy; (C) Visualization of the electrode strain and the probability distributions of the in-plane and out-of-plane components of the deformation field; (D) The kernel density for larger and smaller particles; (E) Amplitude of particle lateral displacement and probability distributions of displacement amplitudes; (F) Localized particle rotation observed through in situ optical microscopy and optical imaging of randomly occurring irregular particle movements; (G) Selected Bragg peaks with different chemomechanical behaviors upon cell cycling; (H) Probability distribution of η for all the captured Bragg peaks and scatter plot of Bragg peak displacements. Adapted with permission^[6]. Copyright 2025, American Association for the Advancement of Science.

To assess whether such behavior persists under practical cell conditions, the authors extend their analysis to a compressed single-layer pouch cell using in situ X-ray laminography^[7]. Three-dimensional tracking of tens of thousands of particles reveals that substantial electrode

strain develops early in the first charging cycle, well before the activation of oxygen redox reactions in Li- and Mn-rich cathodes. Optical-flow analysis uncovers pronounced spatial heterogeneity in the deformation field, with dominant out-of-plane displacement near electrode edges and comparatively weaker in-plane motion toward the interior [Figure 1C]. Particle-size-resolved analysis further shows that smaller particles exhibit systematically larger out-of-plane displacements than their larger counterparts, indicating a size-dependent mechanical response likely arising from faster electrochemical kinetics and enhanced local strain generation [Figure 1D]. Together, these observations highlight the critical role of mechanical mismatch among different cell components and particle populations, demonstrating that electrode deformation is governed not only by active material chemistry but also by microstructural heterogeneity and the mechanical architecture of the full cell stack.

Beyond these gradual deformation modes, Yijin Liu, Juner Zhu, and colleagues identify a previously underappreciated class of sparse, rapid particle-motion events. Statistical analysis reveals that while most particles undergo slow, continuous displacement during charging, a small subset exhibits abrupt, high-velocity rotations and translations [Figure 1E]. Operando optical microscopy confirms that these events correspond to loosely constrained particles that experience sudden mechanical perturbations upon electrochemical activation [Figure 1F]. Although rare, such events represent localized strain-release processes that contribute disproportionately to the heterogeneous evolution of electrode morphology, underscoring the inherently intermittent nature of stress relaxation in composite electrodes.

To elucidate the microscopic origin of these strain dynamics, the authors employ grain-resolved synchrotron x-ray diffraction to decouple chemical and mechanical responses at the crystal-grain level^[8]. By tracking Bragg peak trajectories, they distinguish lattice-spacing changes associated with Li-ion (de)intercalation from tangential peak motion arising from physical grain rotation [Figure 1G]. Statistical analysis of hundreds of grains reveals a broad spectrum of behaviors, including chemically dominated, mechanically dominated, and strongly coupled chemomechanical responses. Notably, a substantial fraction of grains undergoes rotation-dominated motion despite being electrochemically inactive, indicating that stress propagates from chemically active regions into neighboring inactive domains [Figure 1H]. This observation establishes a hierarchical strain-transmission network, in which chemically active grains act as primary stress sources while inactive grains participate by accommodating and relaying transmitted strain.

In summary, this study elucidates the multiscale evolution of “strain cascading” through a multimodal characterization framework. At the microscopic scale, synchrotron X-ray diffraction enables grain-resolution imaging under operating conditions, revealing fundamental coupling between chemical intercalation/deintercalation and physical grain rotation. This demonstrates that strain originates from asynchrony in lattice breathing. These grains serve as primary strain sources, where anisotropic lattice expansion generates local stress fields that propagate to neighboring grains, forming mesoscale propagation. Transmission X-ray microscopy combined with optical microscopy and optical flow analysis under operating conditions reveals collective cluster rearrangement and rapid random particle motion driven by inter-particle charge state heterogeneity. Ultimately, three-dimensional in situ X-ray tomography confirmed that the amplification of these microscopic events dominates macroscopic electrode deformation, manifesting as significant out-of-plane displacement and overall wrinkling. Collectively, these findings reveal a hierarchical trajectory of strain propagation—from individual chemically triggered points to large-scale mechanical degradation. This strain cascade phenomenon resembles dislocation avalanches in crystalline plasticity, shear band propagation in metallic glasses, and domino-like stress transfer in granular media, involving localized activation nodes, threshold-dependent propagation, heterogeneous spatial distribution, and collective asynchronous responses. However, unlike purely mechanical avalanche phenomena, the strain cascade here is jointly driven by electrochemical heterogeneity and mechanical response, introducing asynchronous chemical activation as a triggering mechanism.

Importantly, this framework redefines mechanical fatigue as a collective phenomenon that does not require uniform participation of all active material. Even electrochemically inactive domains contribute to degradation by serving as conduits for stress transmission. These insights carry important implications for battery design, indicating that strategies focused solely on material composition or suppression of lattice expansion may be insufficient to ensure durable operation. Instead, electrodes must be engineered as adaptive, stress-resilient systems, where microstructural design promote controlled particle connectivity, tunable elasticity, and effective dissipation of transmitted stress. By revealing how local electrochemical asynchronicity drives hierarchical mechanical responses, Yijin Liu, Juner Zhu, and colleagues provide a mechanistic foundation for designing next-generation intercalation cathodes with improved structural stability and extended cycle life.

DECLARATIONS

Authors' contributions

Drafted the manuscript: Yan, W.

Revised and rewrote sections of the manuscript: Li, Y.

Availability of data and materials

Not applicable.

Financial support and sponsorship

This work is supported by Wallonia Government in the frame of "Plan de Relance" (2310153-BatFactory) and China Scholarship Council (No. 202406240020).

Conflicts of interest

All authors declared that there are no conflicts of interest.

Ethical approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

Copyright

© The Author(s) 2026.

REFERENCES

1. Park, G.T.; Park, N.Y.; Ryu, J.H.; et al. Zero-strain Mn-rich layered cathode for sustainable and high-energy next-generation batteries. *Nat. Energy* 2025, 10, 1215-1225. DOI: 10.1038/s41560-025-01852-3.
2. Lu, X.; Bertei, A.; Finegan, D.P.; et al. 3D microstructure design of lithium-ion battery electrodes assisted by X-ray nano-computed tomography and modelling. *Nat. Commun.* 2020, 11, 2079. DOI: 10.1038/s41467-020-15811-x.
3. Xiong, J.; Wang, M.; Huang, R.; et al. Recent progress of in-situ/operando characterization approaches of zinc-air batteries. *Chem. Synth.* 2024, 4, 17. DOI: 10.20517/cs.2023.46.

4. Zhang, Y.; Hao, S.; Xiao, X.; et al. Operando chemo-mechanical evolution in $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$ cathodes. *Natl. Sci. Rev.* 2024, 11, nwae254. DOI: 10.1093/nsr/nwae254.
5. Liu, H.; Strobridge, F.; Borkiewicz O.J.; et al. Capturing metastable structures during high-rate cycling of LiFePO_4 nanoparticle electrodes. *Science* 2014, 344, 1252817. DOI: 10.1126/science.1252817.
6. Sun, T.; Qian, G.; Fang, R.; et al. Electrode strain dynamics in layered intercalation battery cathodes. *Science* 2025, 390, 1272-1277. DOI: 10.1126/science.aea2763.
7. Zan, G.; Qian, G.; Gul, S.; et al. In situ visualization of multicomponents coevolution in a battery pouch cell. *Proc. Natl. Aca. Sci. U.S.A.* 2022, 119, e2203199119. DOI: 10.1073/pnas.2203199119.
8. Lin, F.; Liu, Y.; Yu, X.; et al. Synchrotron X-ray Analytical Techniques for Studying Materials Electrochemistry in Rechargeable Batteries. *Chem. Rev.* 2017, 117, 13123-13186. DOI: 10.1021/acs.chemrev.7b00007.

Accepted Article