DynamicsoftheLithiumMetalElectrodeposition:Effects
ofaGasBubble

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Understandingthedynamicsoflithiummetalelectrodepositioniscrucialto
designingsafeandreliablelithiummetalanodes.Inthisstudy,a grand
potential-basedphase-fieldmodelisdevelopedtoinvestigatetheeffectofa
gasbubble(whichformsduetotheternal side reactions)onthedynamics
ofthedendritegrowthduringelectrodeposition.Itisobservedthatwiththe
presenceofastaticgasbubble,thedendritegrowthislargelyaccelerated,
owingtotheaccumulationoflithiumionsonthefarsideofthebubbleaway
fromtheanodesurface,whichcanserveasanion“reservoir”fordendrite
growth,leadingtothetiltingofthelithiumdendrites towardthebubble.
The
effects of the bubble size and distance to the anode are further studied,
demonstratingthatthelargerthebubble size andthecloser to the anode, the
longer the lithiumdendrites will grow. Notably, withamobilebubble, the
dendrite growth can be delayed due to the “stirring effect,” where the motion
ofthebubblecanfacilitatetheionmigration.This effect is maximized when
thebubble moving speed is close to the electrodeposition speed. It is hoped
thatthisstudycanserveasanexampletoexploittheeffectofoextrinsicfactors
onthedendritegrowthdynamics.

1. Introduction

Thereis a continuous trend for the complete electrification of
transportation worldwide,[1–3] to reduce carbon emissions and
tackle environmental challenges such as global warming. A key
requirement for the commercialization of electric vehicles is to increase
theenergy density of lithium batteries. Lithium metaballey, the “holy
grail” for batteries with high specific capacity and energy density,[4–8] remains
one of the most promising solutions. Meanwhile, dendritic growth, the un-
controlled nonlinear growth of metal deposits, is one of the main issues that
couldresultin battery failure and even severe safety issues for the lithium
metal battery.[9–11] Understanding the dendrite growth mechanism during
electrodeposition is vital to design a dendrite-free lithium metal battery.

Another non-negligibleaspect of the degradation of lithium batteries is gas
generation, which occurs due to the complex interplay between the anode,
cathode, and electrolyte.[12–15] For instance, it has been discovered that the
decomposition of carbonate electrolytes

could lead to the formation of multiple gases, including H2, CO,
CH4, C2H6, and CO2,[13,14] whereas the release of O2 from the
lattice oxygen is also observed with ternary cathodes.[15–17] Inpar-
ticular, the carbonate electrolytes could react with the chemically
active lithium metal anode,[18] forming mesoscopic (in the size of
nm to mm) gas bubbles. These bubbles could either stick on the
anode surface or release into the electrolyte, even resulting in the
bulging of a soft pack. Previous theoretical work has shown that
the gas bubble could facilitate the growth of dendrite underneath
the H2 bubble for the Zn battery due to the strong turbulence that
promotes the zinc ion convection.[19] While previous experimen-
tal observation has demonstrated that the formation of these gas
bubbles may hinder the dendrite growth underneath the bubble
andfacilitatethe dendrite growth in thevicinity ofthe bubble.[20]

So far, a comprehensive theoretical understanding of the influ-
ence of extrinsic factors such as a gas bubble (e.g., the influence
of bubble size, bubble position, bubble moving speed, and bub-
ble moving direction) is still lacking.

On that front, phase-field simulations have been widely
adopted to understand the phase transitions, phase transforma-
tions, domain structures, and microstructure evolutions.[21–23] In
particular, it has been widely employed to simulate the morpho-
logical evolution of lithium metal-based anodes.[24–35] These stud-
ies reveal the underline physical insights and critical parameters
for the dendrite growth, which could provide design principles to realize dendrite-free lithium metal batteries.

In this study, a grand potential-based phase-field model is developed to investigate the effect of a gas bubble on the lithium metal electrodeposition kinetics and dendrite growth dynamics during electroplating. It is discovered that the presence of gas bubbles could significantly modulate the dendrite growth pattern, where these bubbles could act as a lithium-ion “reservoir” on the hemisphere external to the electrode. The local lithium enrichment with a static gas bubble gives rise to an additional driving force for the dendrite growth, while also leading to the bending of dendrites. Further studies reveal that the larger the gas bubble, the faster the dendrite growth; whereas the shorter the bubble-anode distance, the quicker the dendrite nucleates. Meanwhile, interestingly, the dendrite growth can be delayed with a moving bubble. This is attributed to a “stirring effect” where the motion of the bubble could lead to the homogenization of the local ion concentration. This study not only highlights the importance of gas bubbles on the electrodeposition kinetics of a lithium metal anode, but also provides an effective and insightful approach to reveal the non-negligible influence of extrinsic factors, e.g., bubbles, and impurities, etc., on the performance of lithium metal batteries.

Following our previous works,[24,31] a grand potential-based phase-field model[16–38] is built where the nonconserved phase-field variable \( \xi \) is introduced as the phase order parameter, where \( \xi = 1 \) and 0 represent the pure electrode and electrolyte phases, respectively. For the sake of simplicity, the mechanical process at the interface is ignored. At room temperature, the kinetic evolution of the order parameter \( \xi \) can be expressed as:

\[
\frac{\partial \xi}{\partial t} = -L_o \left( g' (\xi) - k \nabla^2 \xi \right) - L_h \eta (\xi) + \frac{c_{Li}}{c_0} \exp \left( \frac{-\alpha F \eta}{RT} \right) - \frac{\exp \left( \frac{\mu_m - \mu}{RT} \right)}{1 + \exp \left( \frac{\mu_m - \mu}{RT} \right)} \left[ 1 - h (\xi) \right] [1 - \zeta] \tag{1}
\]

where \( L_o \) and \( L_h \) are the interfacial mobility and electrochemical reaction kinetic coefficient, respectively. \( g(\xi) \) is the double-well function defined by: \( g (\xi) = W \xi^2 (1 - \xi)^2 \). \( W \) is the switching barrier. \( k \) is the gradient coefficient, which is related to the surface tension \( \gamma \) and interfacial width \( \delta \) by \( k = 6 \gamma \delta \). \( h (\xi) \) is the partition function. \( \alpha, F, R, T \), and \( c_0 \) are the charge-transfer coefficient, Faraday constant, gas constant, temperature, and initial Li-ion molar ratio, respectively. \( \eta_a \) is the activation overpotential, which is related to the applied overpotential \( \varphi \), \( \eta_a = \varphi - E^0 \), where \( E^0 \) is the standard equilibrium half-cell potential. To model the gas bubble, an additional non-evolving order parameter \( \zeta \) is introduced, where \( \zeta = 1 \) represents the gas bubble. The lithium-ion concentration \( c_{Li} \) is related to the chemical potential \( \mu \), order parameters \( \xi \) and \( \zeta \), i.e.,

\[
c_{Li} = \frac{\exp \left( \frac{\mu_m - \mu}{RT} \right)}{1 + \exp \left( \frac{\mu_m - \mu}{RT} \right)} \left[ 1 - h (\xi) \right] [1 - \zeta] \tag{2}
\]

where \( \epsilon^i \) is the difference in chemical potential for lithium and the neutral component. The chemical potential can be obtained by solving the coupled electromigration equation, while the electric potential is calculated by solving the conduction equation.[24] The diffusivity inside the gas bubble is set as zero. The detailed derivation of the equations can be found in previous reports[24] and the Supporting Information.

The phase-field equations are solved using the open-source MOOSE framework.[39] A 2D mesh of 200 \( \times \) 200 is employed, with each grid representing 1 \( \mu \)m. The simulation is performed at room temperature (300 K). The Newton method is used as the numerical tool, with the bdf2 scheme and single matrix preprocessing (SMP). Dirichlet boundary conditions are applied along the X dimension (perpendicular to the metal/electrolyte interface) for the phase-field variable \( \xi \), chemical potential \( \mu \), and applied overpotential \( \varphi \), while no flux boundary conditions are applied along the Y dimension (which is perpendicular to the nominal direction of the electric field). The left and right boundaries of the order parameter \( \xi \) are fixed at 1 (metal) and 0 (electrolyte), the chemical potential at both ends is fixed at 0 (fixed concentration for Li species on both sides), and the potential is set to the overpotential applied on the left boundary, and fixed to zero on the right boundary. A schematic diagram of the boundary conditions is given in Figure S1 (Supporting Information). To qualitatively model a moving bubble, a quasi-static bubble motion model is established. The bubble position is out forward stepwise by 20 \( \mu \)m after a certain time \( t \) according to the different moving speeds, as shown in Figure S2 (Supporting Information). The primary simulation parameters before and after normalizations are listed in Table S1 (Supporting Information).

2. Results and Discussion

The lithium electrodeposition process with and without a gas bubble under a relatively high applied overpotential (e.g., \(-0.22 \text{ V}\)) is shown in Figure 1. A 20 \( \mu \)m thick lithium metal anode is set as the initial configuration (Figure 1a). The time-resolved lithium dendrite growth dynamics without the gas bubble are depicted in Figure 1a–d. It can be seen that after deposition for 150 s, the surface instability fluctuation shows up. During the consequent electrodeposition process, the small nuclei grow into several long filaments after 270 s, consistent with previous reports.[24,31] The physical mechanism for the dendrite growth process has been attributed to the complex interplay between diffusion, electromigration, and electrodeposition.[24] Meanwhile, when a gas bubble with a radius of 20 \( \mu \)m is placed inside the electrolyte, i.e., 90 \( \mu \)m away from the initial electrode, as shown in Figure 1e–h, the dynamic behavior of dendrite growth changes dramatically. It can be observed that the electrodeposition is severely hindered for the region shaded by the gas bubble, forming a concave-like structure. Meanwhile, it should be noted that in the case of strong turbulence, an opposite trend can be observed where the dendrite can grow underneath the bubble with ion migration from convection.[19] In a battery with well confined rigid system and limited liquids, in most cases, the turbulence should be minimized. After electrodeposition for 200 s, with the presence of a gas bubble, fewer dendrites can be seen, while the maximum dendrite length is much longer (Figure 1g), which eventually becomes more prominent after 270 s (Figure 1h). It is also interesting to note that, in this case, the dendrites in the vicinity of the bubble tilt toward the bubble, consistent with the previous experiment by in situ optical observations.[20] The tilting of the
dendrite could generate significant internal stress at the root of the dendrite, which may eventually lead to the breakdown of the dendrite and irreversible lithium loss, as has been observed in the previous experiments.\textsuperscript{[20]} To further investigate the physical mechanism for the dendrite growth with gas bubbles, the lithium-ion concentration distribution is plotted, as illustrated in Figure 2. With the presence of a gas bubble, an enrichment of the lithium-ion concentration can be observed on the right side of the bubble (away from the electrode), while the depletion of lithium-ion concentration surrounding the left side of the bubble close to the electrode (Figure 2a). This can be understood since the bubble with zero lithium-ion diffusivity can severely hinder the lithium-ion transport, which causes local ion enrichment/depletion near/away from the lithium-ion source. After electrodeposition for 150 s, it can be discovered that a fan-shaped lithium-ion concentration enrichment area is formed, showing the further increase of lithium-ion concentration on the right side of the bubble (Figure 2b). While the lithium-ion concentration has been depleted in between the bubble and anode. This further prevents the deposition of lithium metal beneath the bubble. Whereas after a longer electrodeposition time, the ion enrichment near the bubble starts to decrease as the dendrites grow longer. This can be understood since an additional transport pathway has been built with the growth of a dendrite, where the far side of the bubble acts as an additional lithium-ion source for the dendrite growth (Figure 2c,d). The line plot of the horizontal and vertical concentration distributions through the bubble center is obtained, as shown in Figure 2e,f. As the deposition time increases, the concentration of the left side of the bubble (close to the anode surface) decreases monotonically; however, on the right side of the bubble far away from the anode, the lithium-ion concentration first increases and then decreases after 150 s (Figure 2e), consistent with the 2D contour plots. While along the vertical direction, the Li-ion concentration decreases monotonically over time, showing the continuous transport of Li-ion through the two sides of a bubble.

In a short discussion, this reveals that the bubble could act as an ion reservoir during the initial deposition stage, which then provides an additional driving force for the consequent dendrite growth process. As a result, the dendrite growth direction tilts toward the bubble region, leading to the bending of dendrites. It should be noted that this effect not only works for gas bubbles but any stuff that could potentially block the lithium-ion transport tunnel, including impurities in the electrolyte/separator, etc.

Having understood the physical insight of the dendrite growth kinetics with a bubble, we proceed to investigate the effect of the bubble size on the electrodeposition. In this study, the bubble center is fixed while the bubble size changes from 4 to 20 \textmu m (Figure 3). As can be expected, when the bubble size is relatively small (e.g., <4 \textmu m), it will not significantly affect the dendrite growth (Figure 3a), after electrodeposition for 270 s, the shape and average length of dendrites are similar to the case without a bubble (Figure 1d). No apparent bending or tilting of the dendrites can be observed. Increasing the bubble size leads to the growth of longer dendrites after the same deposition time, with prominent tilting of the dendrites (Figure 3b,c). The lithium-ion concentrations with different bubble sizes after electrodeposition for 270 s are plotted in Figure 3d–f. It can be seen that as the bubble size increases, the ion enrichment area becomes more

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Figure 1. Microstructure evolution for the lithium metal anode during electrodeposition a–d) without and e–h) with a gas bubble. a) Electrode morphology without a bubble. The initial electrode morphology and after deposition for b) 150 s, c) 200 s, and d) 270 s with an applied overpotential of $-0.22 \text{ V}$. e) Electrode morphology with a bubble. The initial anode morphology with a gas bubble and the morphology after deposition for f) 150 s, g) 200 s, and h) 270 s with an applied overpotential of $-0.22 \text{ V}$. The bubble radius is 20 \textmu m, while the bubble center is 90 \textmu m away from the initial electrode/electrolyte interface.
prominent on the far side of the bubble (away from the anode), while the shaded ion depletion region is also larger, resulting in the tilted growth of the lithium dendrite. This is confirmed by the line plot of the lithium-ion concentration cutting through the bubble center along the horizontal axis (Figure 3g), where the larger the bubble size, the higher the concentration difference between the two sides of the bubble. The dendrite length is further plotted against electrodeposition time for different bubble sizes (Figure 3h), it can be discovered that when the bubble size is larger, the dendrite nucleation time is shorter and the dendrite growth velocity is higher. This can be understood since the lithium-ion “reservoir” becomes larger with a larger bubble, providing a higher additional driving force for the lithium dendrite growth. The effect of bubble density is further investigated (Figure S3, Supporting Information), which suggests that increasing the bubble density could lead to slightly accelerated dendrite growth, which is more severe when the bubbles aggregate. This study also indicates that while the large bubbles are detrimental to the electrodeposition, the smaller bubbles (with a radius <4 μm) could have a moderate effect, and the effect of bubble size is more prominent as compared to the bubble density. It is suggested that practically, the control of the bubble size is key to effectively reducing the side effect of a gas bubble, which can be achieved either by reducing the gas reactions from the gas production side, as well as active perturbations during battery electrodeposition that could destabilize the large bubbles.

The relative position of the bubble is also another critical aspect that could also affect the dendrite growth. The morphology of the Li metal anode after electrodeposition for 135 s with different bubble positions is given in Figure 4. The bubble center is fixed at 60, 80, and 120 μm from the left edge of the initial anode position, while the bubble size is fixed at 20 μm. As shown in Figure 4a–c, the dendrite length is longer when the bubble is closer to the anode surface. This is also confirmed by the line plot of the dendrite length with respect to the electrodeposition time for different bubble-anode distances (Figure 4d). The kinetic evolution process of the anode surface for different bubble positions is given in Figure S4 (Supporting Information). It can be observed that when the distance is 60 μm, the dendrite nucleates near the two edges of the bubble on the anode surface, which grow into two long filaments that tilt toward the bubble, and after surpassing the bubble region, the growth direction becomes straight. The initial degree of tilting for the dendrites decreases with increasing bubble-anode distance. While for the case when the bubble is placed 140 μm to the anode surface, a more stable electrodeposition process can be discovered. To understand the mechanism behind the dendrite growth rate and bubble-anode direction, the contour plots (Figure S5, Supporting Information) and line plots (Figure 4d–g) of the ion concentrations after different deposition times (10, 70, and 140 s) are given. It can be observed that while the concentration on the right side of the bubble is similar, the concentration decay on the left side of the bubble is more severe for the case when the bubble anode distance is shorter. After 140 s, the lithium-ion on the left side of the bubble almost drained for the case when the bubble is very close to the anode (Figure 4g). The significant differences in lithium-ion concentration between the bubble-shaded and free surface could result in the variation of the local plating rate, giving rise to
to preferred nucleation sites near the edge of the region shaded by the bubble. This effect is less severe when the bubble is further away from the anode surface. Briefly, the bubbles that stick on the anode surface are detrimental to the reversibility of the plating/stripping, while the bubbles in the middle of the electrolyte have a minimal effect. Reducing the bubble adhesion on the anode surface is another effective way to suppress dendrite nucleation and growth. This can be achieved by adding defoamers on the electrolytes, etc.

The effect of a moving bubble on the electrodeposition kinetics is further revealed in Figure 5. For comparison, two cases are presented: deposition with a relatively high (e.g., 0.67 μm s⁻¹, Figure 5a–c) and medium bubble moving speed (e.g., 0.4 μm s⁻¹, Figure 5d–f). To ensure consistency with the discussion of static bubbles, we set the starting position of the moving bubbles to be identical to the bubble position in Figure 1, i.e., coordination (110, 100) in the 2D simulation system, as marked by the dashed black circle. It can be observed that at the initial stage, after deposition for 100 s, the electrodes are relatively flat for both cases. After a longer deposition time (e.g., 200 s), two distinctly different scenarios can be observed: with a faster bubble moving speed, the bubble has moved out of the electrolyte after 200 s, and the surface perturbation becomes more prominent (Figure 5b) as compared to the case with a slower bubble moving speed (Figure 5e);
while interestingly, the dendrite growth is greatly suppressed under slower bubble moving speed (0.4 μm s⁻¹, Figure 5f) as compared to the case without a gas bubble (Figure 1d). Eventually, after 286 s, the dendrites grow much longer with a faster bubble moving speed (0.67 μm s⁻¹, Figure 5c). To further highlight the “stirring effect” from a gas bubble, the lithium-ion concentration distributions with a static bubble and a moving bubble at a speed of 0.4 μm s⁻¹ are further plotted in Figure S6 (Supporting Information). It can be found that the moving bubbles could act as a “stirrer” which homogenizes the local lithium-ion concentration when it moves. For a direct comparison, we extract the lithium-ion concentration difference on the left and right sides of the bubble, as shown in Figure S6g (Supporting Information). It can be seen that when the bubble is stationary, the concentration difference between the left and right ends of the bubble continues to increase. However, when the bubble moves, the concentration difference between the left and right ends of the bubble decreases, and the faster the bubble moves, the “stirring effect” is more obvious. This result provides direct evidence for the existence of the “stirring effect,” as well as detailed explanations for the dendrite
Figure 5. Microstructural evolution of lithium metal anodes during electrodeposition with different bubble moving speeds. Morphological evolution of anode with bubbles moving at a–c) 0.67 μm s⁻¹ and d–f) 0.4 μm s⁻¹. The initial bubble position is marked by the dashed circle. g) The dendrite length as a function of deposition time under different bubble moving speeds. h) Comparison of the dendrite lengths after electrodeposition for 220 s, under different bubble moving speeds.

In addition, the initial surface roughness will also affect the dendrite growth behavior and underline mechanism. We have conducted two sets of simulations to investigate the interactions between a lithium protrude and a gas bubble by varying the location of a bubble with respect to an initial lithium protrude (as shown in Figures S7 and S8, Supporting Information). From Figure S7 (Supporting Information), it can be observed that when the bubble is located right above the lithium protrudes, it will inhibit the growth of dendrites. This can be understood since the lithium-ion transport to the protrudes is inhibited. As the bubble progresses toward the right, the growth rate of dendrites decreases, and the inhibitory effect weakens. However, for comparison, when the bubble is placed at a distance from the protrudes, it will promote the growth of dendrites (Figure S8, Supporting Information), similar to what we have discussed in the main text. While a moving bubble will reduce the dendrite growth rate. This study reveals that the lithium dendrite growth can also be
inhibited when the bubble moves to the top of the protrudes, and the “stirring effect” is solid when the bubble is not placed directly on the top of the protrudes. When the bubble moves along the metal surface, as shown in Figure S9 (Supporting Information), the growth rate of dendrites is reduced, but the reduction effect is much weaker than that of the vertical movement as discussed in the main text. It is also interesting to note that in this case the dendrites will nucleate and grow close to the opposite of the bubble moving direction.

3. Conclusion
In conclusion, we have developed a grand potential-based phase-field model to investigate the effect of a static and moving gas bubble on the lithium dendrite growth dynamics. It is revealed that the presence of a static gas bubble causes significant dendrite growth, where the bubble side external to the electrode acts as a lithium-ion “reservoir”. It provides an additional driving force for the dendrite growth, leading to the tilting of the dendrite toward the bubble. While the drain of the lithium-ion on the regions shaded by the bubble could lead to uneven growth on the metal anode, acting as the preferred nucleation sites near the bubble edges. It is further revealed that a larger and closer-to-anode bubble triggers the growth of longer dendrites with a shorter nucleation time. However, a moving bubble could delay the dendrite growth, which shows minimum dendrite length at a speed of ≈0.4 μm s⁻¹ (which is close to the electrodeposition speed in this study). This can be attributed to the “stirring effect” where the moving bubble can homogenize the lithium-ion concentration. The competition between the “stirring effect” and “reservoir effect” gives rise to an optimum bubble moving speed for dendrite suppression. This finding provides promising engineering solutions for stabilizing lithium metal batteries by decreasing the bubble size, removing those bubbles near surfaces, or engineering the bubble moving speed. In a real battery system, the presence of gas bubbles can be indirectly and effectively monitored using a gas sensor, which has been a standard technique in the field nowadays. Practically, the number and size of bubbles can be controlled by adding surfactant or deformer in the electrolyte, while the movement of the bubble can be tuned by applying external stimuli during battery charging, such as local vibration of the battery, magnetic forces, or ultrasonic wave. Then, the moving speed of the bubbles can be controlled by adjusting the frequency and power density of the vibration and ultrasonic wave. This study, although theoretical in nature, provides concrete design principles for the design of dendrite suppression batteries. We hope this study could spur further theoretical/experimental efforts in the complicated interactions between dendrite growth and extrinsic factors such as gas bubbles.

Supporting Information
Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest
The authors declare no conflict of interest.

Data Availability Statement
The data that support the findings of this study are available from the corresponding author upon reasonable request.

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[27] D. Ely, A. Jana, R. Garcia, J. Power Sources 2014, 272, 581.
[28] L. Chen, H. Zhang, L. Liang, Z. Liu, Y. Qi, P. Lu, J. Chen, L. Chen, J. Power Sources 2015, 300, 376.
[29] V. Yurkiv, T. Foroozan, A. Ramasubramanian, R. Shahbazian-Yassar, F. Mashayek, Electrochim. Acta 2018, 265, 609.
[30] V. Yurkiv, T. Foroozan, A. Ramasubramanian, R. Shahbazian-Yassar, F. Mashayek, MRS Commun. 2018, 8, 1285.
[31] Z. Hong, V. Viswanathan, ACS Energy Lett. 2019, 4, 1012.
[32] Q. Wang, G. Zhang, Y. Li, Z. Hong, D. Wang, S. Shi, NPJ Comput. Mater. 2020, 6, 176.
[33] Z. Mu, Z. Guo, Y. Lin, Energy Storage Mater. 2020, 30, 52.
[34] R. Zhang, X. Shen, Y. Zhang, X. Zhong, H. Ju, T. Huang, X. Chen, J. Zhang, J. Huang, J. Energy Chem. 2021, 47.
[35] Z. Yao, C. Chen, C. Li, J. Hou, J. Zhang, L. He, Y. Yang, X. Xia, J. Xiong, ACS Appl. Energy Mater. 2021, 4, 10380.
[36] M. Plapp, Phys. Rev. E 2011, 84, 031601.
[37] S. Jin, Y. Wu, H. Yang, Y. Huang, Z. Hong, STAR Protoc. 2022, 3, 101713.
[38] D. Gaston, C. Newman, G. Hansen, D. Lebrun-Grandié, Nucl. Eng. Des. 2009, 239, 1768.
[39] M. Tonks, D. Gaston, P. Millett, D. Andrés, P. Talbot, Comput. Mater. Sci. 2012, 51, 20.
[40] Z. Wang, L. Zhu, J. Liu, J. Wang, W. Yan, Energy Fuels 2022, 36, 6038.
[41] T. Cai, P. Valecha, V. Tran, B. Engle, A. Stefanopoulou, J. Siegel, eTransportation 2021, 7, 100100.
[42] S. Nahidi, I. Gavzan, S. Saedodin, M. Salari, B. Maddah, J. Electrochem. Soc. 2020, 167, 120524.
[43] K. Wang, P. Pei, Y. Pei, Z. Ma, H. Xu, D. Chen, Sci. Rep. 2016, 6, 21068.
[44] Y. Asakura, K. Yasuda, Ultrason. Sonochem. 2022, 82, 105890.