A Preliminary Study on EG Films Using MD Simulation

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ABSTRACT

Advances in battery technology have highlighted the need for strong thermal management to prevent thermal runaway in high-performance energy storage systems such as lithium-ion batteries. Expandable Graphite (EG), which expands at high temperatures to provide insulation and flame retardancy, is attracting attention as a promising heat-blocking material between battery cells. In this study, we investigate the thermal conductivity and expansion properties of EG to evaluate its effectiveness as a heat-blocking material. Using MD simulation, we predict the expansion mechanism of EG at high temperatures and evaluate the impact of structural changes on thermal performance. Based on our findings, we design an experiment to measure the thermal conductivity of EG under various conditions. Our findings indicate that a decrease in EG particle size and an increase in concentration lead to a reduction in thermal conductivity, thereby enhancing the thermal barrier function of EG. Additionally, laser treatment amplifies expansion and surface porosity, significantly improving thermal stability. These results suggest that EG could become an effective thermal barrier in battery thermal management systems.

KEY WORDS

Expandable graphite(EG), Thermal Conductivity, Molecular Dynamics Simulation

1. INTRODUCTION

With the rapid advancement of battery technology, particularly in lithium-ion systems, effective thermal management has become increasingly critical. Recent innovations in battery design aim to increase energy density, enhance charging speeds, and improve safety, all of which drive the need for advanced thermal management solutions. For instance, high-nickel cathodes and silicon anodes are being developed to maximize energy density, enabling electric vehicles to achieve longer driving ranges and energy storage systems (ESS) to handle greater capacity. However, these advancements have also amplified safety challenges, especially with the risk of thermal runaway, which, if uncontrolled, leads to catastrophic failures (Wang et al., 2012; Doughty & Roth, 2012).

One promising solution to these challenges is the application of thermal barrier materials, such as Expandable Graphite (EG). EG exhibits unique thermal characteristics, expanding rapidly at elevated temperatures to create a porous structure that effectively reduces thermal conductivity. This expansion can create an insulating barrier between battery cells, limiting thermal transfer and potentially preventing the spread of thermal runaway. Recent studies have shown that EG can limit thermal conductivity under high-temperature conditions, making it an ideal candidate for improving the thermal stability and safety of advanced battery systems (Li et al., 2017; Wang et al., 2019).

This study aims to systematically evaluate EG's thermal performance across a range of temperatures and treatments to assess its effectiveness as a thermal management material in high-performance energy storage systems. Using molecular dynamics (MD) simulations, we analyze the high-temperature expansion behavior of EG, while experimental validation examines thermal insulation performance across various EG concentrations and particle sizes. We hypothesize that certain concentrations and particle sizes of EG will yield optimal thermal insulation.

Our findings provide significant insights into EG's role as a safety-enhancing material for next-generation battery systems, highlighting its potential to mitigate thermal runaway and improve battery safety standards. By clarifying EG’s applicability in thermal management, this study contributes to safer, higher-performance energy storage systems, advancing both battery safety and energy storage technology.

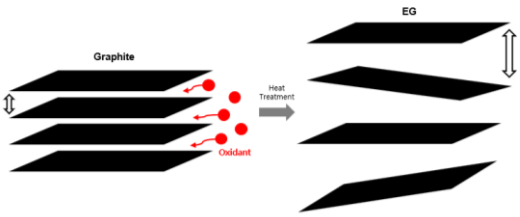

Fig. 1. Expandable Graphite(EG) Schematic Diagram

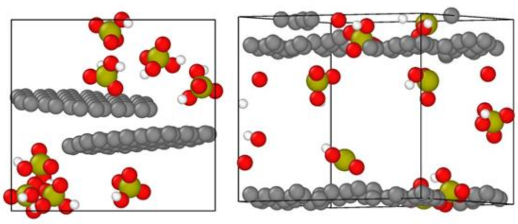

Fig. 2. MD Simulation results of EG

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