

The 14th Asian Coating Workshop 2024

Date May 8 - 10, 2024

Place Vision hall (6th floor), ISC Building,
LG Science Park, 30 Magokjungang 10-ro,
Gangseo-gu, Seoul, South Korea



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1. Committee and organization	03
2. Program at glance	05
3. Conference schedule	06
4. Professor Session	07
5. Oral Session	20
6. Poster Session	35

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Name	Affiliation	Country
Hyun Wook Jung	Korea University	Korea

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Program at glance

The 14th Asian Coating Workshop 2024
May 8 - 10, 2024, Seoul, South Korea

	5/8 WED. (Day 1)	5/9 THU. (Day 2)	5/10 FRI. (Day 3)
Morning		Professor session	Experience Activities
Afternoon	Arrival in Seoul	Short Oral & Poster Session	Luncheon & Farewell
Evening	Registration & Welcome Reception	Banquet & Award Ceremony	

Conference schedule

The 14th Asian Coating Workshop 2024
May 8 - 10, 2024, Seoul, South Korea

Time	24-05-08 (Wed.)	24-05-09 (Thu.)	24-05-10 (Fri.)
8:50		Opening remark (08:50-09:00)	
9:00		Professor session (09:00-12:30) *Poster put-up during coffee break time	LG Chem's R&D activities for the future : R&D of Platform Tech. center <i>Project Leader, Ki Hwan Kim</i> (09:00~09:30)
9:30			
10:00			
10:30			
11:00			
11:30			
12:00			LG Science Park Tour & Outdoor activity - Seoul Botanic Park - (09:30-12:30)
12:30		Lunch (12:30-13:30)	Lunch & Farewell (12:30-14:00)
13:00		*Group photo before lunch	
13:30			
14:00			
14:30		Oral session (13:30-16:15)	
15:00			
15:30			
16:00			
16:30		Poster session (16:15-17:45)	
17:00			
17:30	Registration & Welcome Reception (17:00-19:30)	Move to banquet place (17:45-18:00)	
18:00			
18:30			
19:00			Banquet & Award ceremony *Lucky draw (18:00-20:00)
19:30			
20:00			

Professor session

The 14th Asian Coating Workshop 2024
May 8 - 10, 2024, Seoul, South Korea

Location : Vision Hall (6th floor)

Time	No.	Title	Professor
Professor session I (Session chair : Prof. Hyun Wook Jung)			
09:00-09:15	PO-1	Mass transfer in drying emulsions	Susumu Inasawa (Tokyo Univ. of Agriculture and Technology)
09:15-09:30	PO-2	Near-wall orientational dynamics of rod-like particles in confined shear flows: Couette and Poiseuille flows	Byoungjin Chun Hyun Wook Jung (Korea Univ.)
09:30-09:45	PO-3	Recent Advances in Printing Material Formulation	Ying-Chih Liao (National Taiwan Univ.)
09:45-10:00	PO-4	Recent research topics on the preparation process and microstructural analysis of slurries at Kobe University	Yoshiyuki Komoda (Kobe Univ.)
10:00-10:15	Coffee break & Poster put-up		
Professor session II (Session chair : Prof. Ying-Chih Liao)			
10:15-10:30	PO-5	Research Progress of Microstructures and Smart Process Laboratory	Dongjae Kim (Soonchunhyang Univ.)
10:30-10:45	PO-6	Recent advancement in numerical modeling for particle-laden fluids with wide particle size distribution	Yi-Ju Chou (National Taiwan Univ.)
10:45-11:00	PO-7	Instability in directional solidification of UV-curable coating	Masato Yamamura (Kyushu Institute of Tech.)
11:00-11:15	PO-8	Numerical investigation of flow and mixing behavior of thixotropic fluids	Seon Yeop Jung (Dankook Univ.)
11:15-11:30	Coffee break		
Professor session III (Session chair : Prof. Susumu Inasawa)			
11:30-11:45	PO-9	On the recent development of microfluidic technology for the new coating applications in the National Taiwan University	An-Bang Wang (National Taiwan Univ.)
11:45-12:00	PO-10	Coalescence of particle-coated oil droplets owing to evaporation of a continuous water phase	Kohei Abe (Okinawa Institute of Sci. and Tech.)
12:00-12:15	PO-11	Rheology study of complex fluids using mesoscale simulations and its application towards the process relevant energy storage materials	Young Ki Lee (Hankyong National Univ.)
12:15-12:30	PO-12	Value Chains among University, Chemical Company, and Industrial Machine Company	Kentaro Taki (Kanazawa Univ.)
12:30-13:30	Group photo & Lunch		

Mass transfer in drying emulsions

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Abstract

Drying of complicated fluids is of importance in production processes. Among them, emulsions that consist of liquid droplets suspended in another immiscible liquid are used in variety of fields such as foods or cosmetics. In our laboratory, we have been studying drying of emulsions. Some of our findings are (1) drying kinetics of water droplets immersed in oil (water-in-oil (W/O) emulsions) is explained by diffusion limited process of dissolved water in oil [1,2], (2) phase transfer of amphiphilic molecules such as surfactant from evaporating water to the surrounding oil impedes the rate of water evaporation, especially in the last stage of drying [3]. We will discuss those points in our talk.,

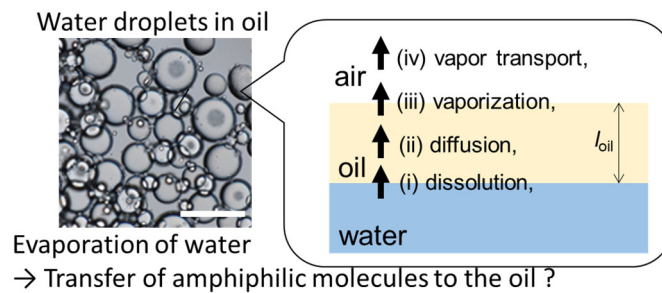


Figure 1 (Left) Optical microscope image of W/O emulsion and (Right) schematic illustration of mass transfer of water through an oil layer. The scale bar in the image is 200 micrometers.

Keywords: water-in-oil (W/O) emulsions, drying of water droplets, phase transfer of molecules

References

- [1] H. Miyazaki and S. Inasawa, *Soft Matter*, **13**, 8990 (2017)
- [2] K. Abe and S. Inasawa, *Langmuir*, **37**, 219-229 (2021)
- [3] K. Hasegawa and S. Inasawa, *Int. J. Heat Mass Transfer*, **208**, 124053 (2023)

Near-wall orientational dynamics of rod-like particles in confined shear flows: Couette and Poiseuille flows

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Abstract

The orbital motion of ellipsoids under a simple shear flow, studied by Jeffery [1] about 100 years ago, has served as the foundation for various subsequent studies on the orientational dynamics of non-spherical particles in diverse shear flows. Even in later research considering additional factors such as orbital diffusion, nonlinear flow profiles, and fluid inertia, Jeffery's solutions have been shown to be applicable with some modifications. However, unlike the extensive research on orientational dynamics in unbounded flows, the motion of non-spherical particles through narrow channels, frequently encountered in coating flows, remains under-explored. Experimental studies in channel flows have revealed non-Jeffery behaviors like pole-vaulting [2], swinging [3], and perpendicular orientation of rod-like particles to the flow direction [4], which are not yet fully understood. To understand how these unexpected near-wall motions arise due to hydrodynamic interactions with a wall, we performed a numerical analysis using the lattice Boltzmann (LB) method. We observed a gradual transition from the Jeffery to non-Jeffery motions as the particle center approaches the wall. Furthermore, we identified the significant differences in near-wall alignment under two common types of shear flows, Couette and Poiseuille flows, and discussed the underlying factors causing these discrepancies.

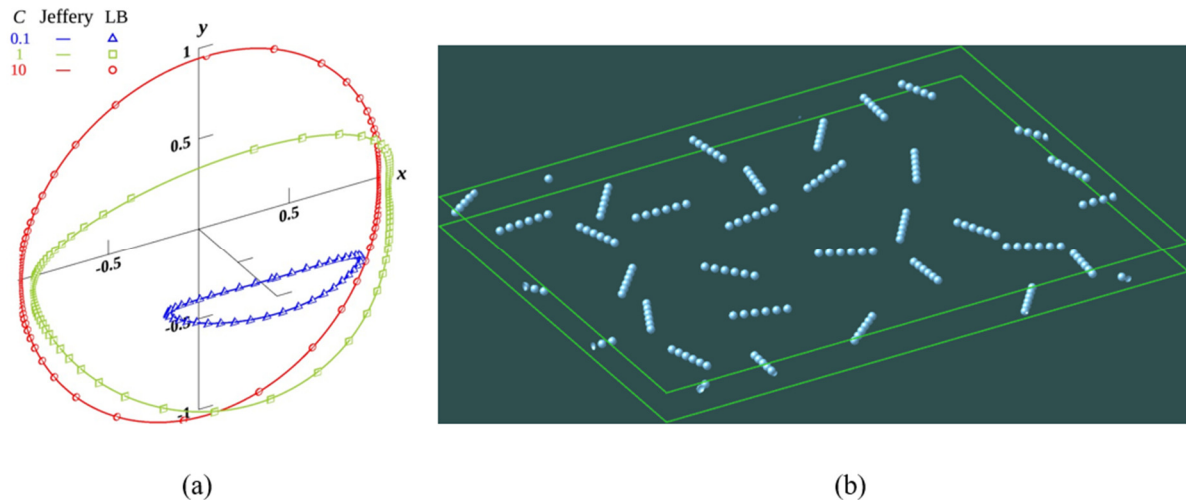


Figure 1. (a) Jeffery's orbits observed far from the wall, and (b) schematic diagram for simulating suspensions of rod-like particles under Couette and Poiseuille flows.

Keywords: rod-like particle, orientation dynamics, lattice Boltzmann, CNC, short fiber

References

- [1] G. B. Jeffery. *The motion of ellipsoidal particles immersed in a viscous fluid*. Proc. R. Soc. London. Ser. A, 102, 161–179 (1922).
- [2] C. A. Stover and C. Cohen. *The motion of rodlike particles in the pressure-driven flow between two flat plates*. Rheol. Acta, 29, 192–203 (1990).
- [3] T. Kaya and H. Koser. *Characterization of hydrodynamic surface interactions of Escherichia coli cell bodies in shear flow*. Phys. Rev. Lett., 103, 138103, (2009).
- [4] A. Carlsson, F. Lundell, and L. D. Soderberg. *Fiber orientation control related to papermaking*. J. Fluids Eng., 129, 457–465 (2007).

Recent Advances in Printing Material Formulation**Ying-Chih Liao^{1*}**¹ Department of Chemical Engineering, National Taiwan University, Taipei, 10617 Taiwan

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Abstract

The recent development in precision printing technology at Chemical Engineering Department, National Taiwan University in 2022 – 2024 will be summarized in this presentation. First, we will examine recent advancements and challenges in the production of low-reflow temperature solder paste with superior physical properties. Additionally, innovative methodologies have been developed to improve the ductility, transparency, and mechanical properties of bacterial cellulose to replace non-biodegradable plastic as printing substrates. Also, biopolymer composites synthesized using eco-friendly methods are fabricated into humidity sensors with low detection limits. Last but not least, for semiconductor packaging applications, a novel model has been developed to facilitate the incorporation of an ultra-high volume of particles within composites, effectively overcoming the processibility limitation arising from high viscosity. Achievement of exceptional composite properties including enhanced thermal conductivity, mechanical strength, and Dk/Df values showcase the excellent performance of the model.

Recent research topics on the preparation process and microstructural analysis of slurries at Kobe University

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Abstract

Slurry, a mixture of particles and solutions, is widely used in the manufacturing processes of various products, including electronic devices. Battery electrodes are one of the most fascinating research fields since the internal structure of the slurry significantly alters cell performance. Recently, higher active material content and lower conductive additive content have been required simultaneously while suppressing the viscosity increase and keeping sufficient electroconductivity. Catalyst layers of fuel cells are also produced by coating and drying the slurry of catalyst particles. Although the slurry is usually less viscous, the dispersion state of ionomers, which is affected by solvent composition, significantly affects the internal structure of the catalyst slurry. Multi-layer ceramic capacitors have a sandwich structure of dielectric and inner electrode layers. Both layers are produced from different slurries, but either requires highly accurate thickness and flatness control. The dispersion state of particulate materials and the change through the manufacturing process need to be studied. In the integrated circuit packages manufacturing process, silica-dispersed epoxy resin filled the gap between the IC tip and wafer by a capillary coating process. Preparing highly condensed but less viscous silica-filled resin is a challenging topic. Although our research group also investigates the coating and drying process of the aforementioned slurry, this talk will focus on recently conducted results on analyzing the preparation process and internal structure of the slurry.

Rheology is the most powerful tool for revealing the dispersion state of particles in the slurry since elastic response provides information on the network structure of particles formed in the slurry and the apparent volume fraction of particles alters the viscous term. This talk will demonstrate the significance of relative viscosity in complicated slurries [1]. We are ambitious in developing novel techniques and approaches for evaluating the internal structure of various kinds of slurry. Rheo-impedance technique can provide significant insights into conductive paths with various length scales [2]. One of the interesting findings is the conductive paths in LiB cathode slurry and the structural change with shear application. Time-domain NMR detects the relaxation process of protons excited by magnetic resonance and can investigate the difference in the adsorption layer over-dispersed particles using a relaxation time as an index [3]. I will explain an example of the combined analysis of TD-NMR and impedance measurement for CNT dispersions. The significance of cryo-TEM observation for validating the internal structure analysis will also be discussed.

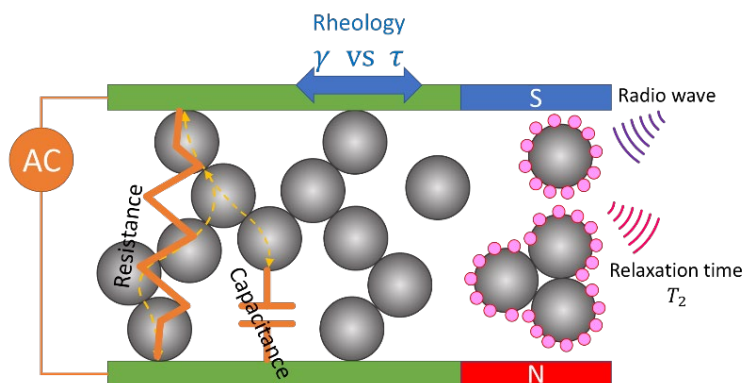


Figure 1. Multifaceted evaluation method of the internal structure of slurries

Keywords: Slurry, Rheology, AC Impedance, TD-NMR

References

- [1] Komoda, Y., *et al.*, *JCIS Open* 5 (2022): 100038.
- [2] Yoshida, K., Komoda, Y. *et al.*, 12th Asia Coating Workshop, Kanazawa (2022)
- [3] Komoda, Y., *et al.*, *Colloids and Surfaces A: Physicochem. and Eng. Aspects* 683 (2024): 133064

Research Progress of Microstructures and Smart Process Laboratory

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Abstract

Microstructures and Smart Process Laboratory was started in September 2022 at Soonchunhyang University. Currently, our laboratory mainly works on rheological analysis for anode battery slurry, machine learning or data mining for various data, and microstructural analysis for coating processes. In addition, we are currently interested in carbon capture, mineralization, and fluidization reactor modeling.

In this presentation, we would like to introduce our past, present, and future research topics related to the coating process. The contents include analysis of a transparent conductive film composed of nanowires, microstructural analyses of a battery anode, a slot coating process, and rheological analysis of a battery anode slurry.

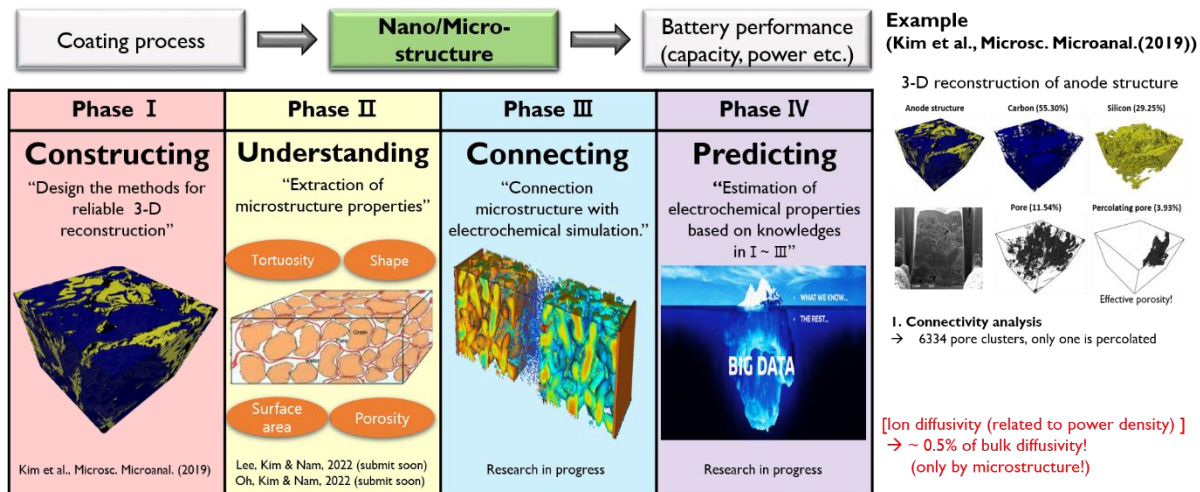


Figure 1. Example of microstructural analyses on battery anode.

Keywords: Coating process, Battery electrode slurries, Microstructural analysis

Recent advancement in numerical modeling for particle-laden fluids with wide particle size distribution

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Abstract

Particle-laden flows are integral to numerous coating technologies, with powder coating being a prime example, which typically requires a diverse particle size distribution. However, accurately predicting solid-fluid flows in such complex scenarios poses significant computational challenges due to the varied numerical treatments required for different particle sizes. In this presentation, I will unveil our recent advancements in a numerical model designed to address this issue through fully coupled simulation of solid and fluid phases. Our model comprises three components tailored to small, median, and large-sized particles, respectively. Small-sized particle motion is simulated using the traditional CFD-DEM approach, leveraging a particle-in-cell methodology with a linked-list data structure for efficient handling of massive particles. Flow around large-sized particles is captured using the immersed boundary method, known for its ability to accurately capture wake flows around moving particles. For median-sized particles—those closely matching grid cell sizes—we introduce a force-partitioning method, effectively distributing momentum and mass feedback into the grid cells. Illustrative simulations of particle mixtures with varying sizes will be presented, along with insights into our ongoing model development efforts.

Instability in directional solidification of UV-curable coating

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Abstract

We show a photo-induced phase separation (PIPS) method to create anisotropic columnar pores in UV-curable acrylic coatings. Upon photo irradiation on the bottom surface of a solvent-initiator-monomer ternary liquid film, a directional solidification proceeds to promote an interfacial instability at the reaction front, resulting in columnar structures that periodically align along the surface. Fig. 1 shows a schematic time-evolution in the structure formation. The photo polymerization reactions proceed in the vicinity of bottom surface as the photo intensity decays along the irradiation direction (regime I). The polymer network develops when the monomer conversion exceeds a critical value, leading to form an un-reacted layer on top of a reacted (solidified) layer (II). The interface between the two layers moves as the solidified layer thickens. Simultaneously, the stress development in the reacted layer induced a non-Fickian diffusion that squeeze out the solvent molecules toward the interface^[1] as so ice crystals in a freezing colloidal suspension reject particles^[2-3]. When the light adsorption coefficient of the polymer is smaller than that of the monomer, the speed of moving interface increases as increasing the monomer conversion, giving rise to a possible interfacial instability above a critical speed (III). The interfacial perturbation grows in amplitude, leaving grooves filled with the solvent insoluble with the polymer (IV). The subsequent solvent evaporation from the grooves creates polymer columns that extend in the direction of photo irradiation (V). Our supplemental experiments revealed that the column orientation was tunable by an inclined photo irradiation.

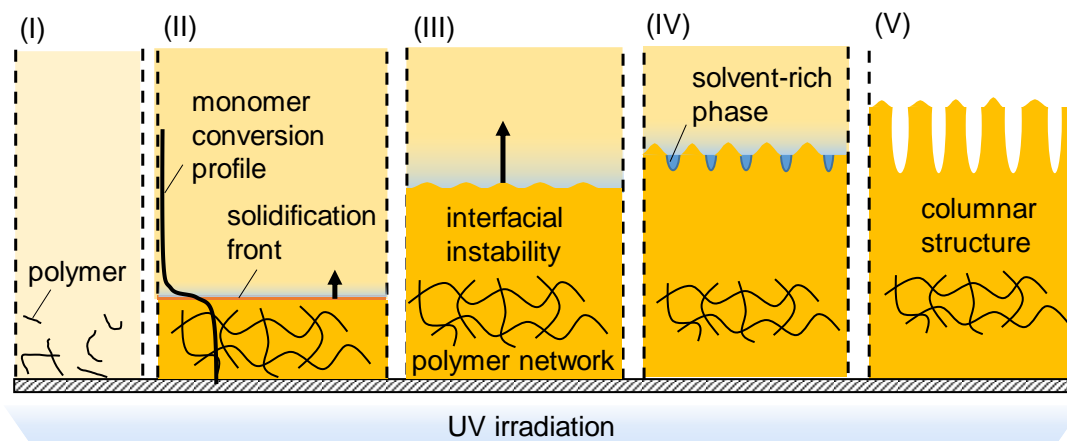


Figure 1 Schematic time-evolutions of columnar structures in the cross section of UV-curable coating

Keywords: UV curing, photo-induced phase separation, interfacial instability, directional solidification

References

- [1] M. Yamamura, Reaction-driven solvent transport in UV-curable phase-separating coatings, *Journal of Coatings Technology and Research*, 20, 15-26 (2023).
- [2] W.W. Mullins, R. F. Sekerka, Stability of a planar interface during solidification of a dilute binary alloys, *Journal of Applied Physics*, 35, 444-451 (1964)
- [3] J.S. Langer, Instability and pattern formation in crystal growth, *Review of Modern Physics*, 52, 1-28 (1980)

Numerical investigation of flow and mixing behavior of thixotropic fluids

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Abstract

Thixotropy refers to a non-Newtonian fluid property where the viscosity of the fluid decreases due to the breakdown of its microstructure when subjected to constant shear force [1]. It is also known as time-dependent shear thinning behavior, observable in paints and coatings [2]. These substances exhibit relatively high viscosity when at rest, but their viscosity decreases over time when subjected to stirring or agitation. An important aspect is the reversibility of this viscosity reduction, meaning that the viscosity returns to its original high value when stirring ceases and the fluid comes to rest. It occurs because the viscosity is governed by their microstructure, which undergoes reversible breakdown and recovery in response to applied shear force.

In this talk, we outline our recent numerical studies on the flow and mixing behavior of thixotropic fluids, along with future research directions. The structure-kinetics model, employed in these studies, describes the microstructure of thixotropic fluids using a structure parameter, λ , which represents the degree of local structure [3]. To provide representative examples, several numerical investigations focusing on the flow and mixing behavior of thixotropic fluids in static mixers have been conducted, including the barrier-embedded partitioned pipe mixer (BPPM) [4], the staggered-herringbone mixer (SHM) [5], Kenics mixer, and the Sulzer SMX mixer. Since each static mixer is designed under different mixing principles, the dependency of mixing performance on the thixotropy parameters varies with the mixer geometry. We explore how different mixing principles in static mixers affect the relationship between thixotropy parameters and mixing performance.

Keywords: Thixotropy, structure-kinetics model, microstructure, static mixer, complex fluids

References

- [1] H.A. Barnes, *Thixotropy—a review*. J. Nonnewton. Fluid Mech., 70, 1-33 (1997).
- [2] A. Marrion, *The Chemistry and Physics of Coatings*, 2nd ed., Royal Society of Chemistry, Cambridge, United Kingdom (2004).
- [3] R.G. Larson, Y. Wei, *A review of thixotropy and its rheological modeling*. J. Rheol., 63(3), 477-501 (2019).
- [4] S.Y. Jung, J.E. Park, T.G. Kang, J.D. Park, *Flow and mixing analysis of a thixotropic fluid in a barrier-embedded partitioned pipe mixer (BPPM): A numerical study*. Int. J. Heat Mass Transf., 184, 122310 (2022).
- [5] J.E. Park, T.G. Kang, S.Y. Jung, *The impact of thixotropic behavior on microfluidic mixing in a staggered-herringbone mixer*. Phys. Fluids, 36(4), 042008 (2024).

On the recent development of microfluidic technology for the new coating applications in the National Taiwan University

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Abstract

Microfluidics bring significant advantages in various applications and is an engaging technology for different industry applications, e.g., chemical reaction, process control and bio-medical detection etc., in the recent years. In this talk, the development of microfluidic components and integration systems for industrial applications will be reported. Special efforts will be focused on the microfluidic applications in the life science studies and clinical diagnoses with the advantages of fast, easy use, and excellent cost performance for biomedical diagnosis testing. An extremely material- and time-saving microliter-TDC (Thin-film Direct Coating) platform [1-3] for fast immunoassay and detection, e.g., the fast TDC WB (western blotting) strip and fast TDC IHC (Immunohistochemistry) was developed to extend the traditional coating field and tested for the practical use and future commercialization [4].

Keywords : Microfluidics, System integration, Miniaturized compact coating system, Thin-film Direct Coating, Biomedical diagnosis

References

- [1] Yen, Y.-K., Jiang, Y.-W., Chang, S.-C., & Wang, A.-B. (2014), Western blotting by thin-film direct coating. *Analytical chemistry*, 86(10), 5164-5170.
- [2] Liu, C.-Y., Lu, D.-C., Jiang, Y.-W., Yen, Y.-K., Chang, S.-C., & Wang, A.-B. (2016), Easy and fast western blotting by thin-film direct coating with suction. *Analytical chemistry*, 88(12), 6349-6356.
- [3] Hsiao, C.-C., Chiang, Y.-W., Chao, T.-L., Tsai, Z.-U., Wang, T.-X., Jiang, Y.-W., Hsu, H.-F., Lu, D.-C., Wang, J.-T., Wang, J.-R., Wang, A.-B., Chang, S.-Y., Chang, S.-C. (2023), *Applied Microbiology and Biotechnology*, 106(24): 8183-8194.
- [4] Desire, C. T., Arrua, R. D., Strudwick, X. L., Allison J., Kopecki, Z., Cowin, A.J., Hilder, E. F. (2023), The development of microfluidic-based western blotting: Technical advances and future perspectives, *Journal of Chromatography A*, 463813.

Coalescence of particle-coated oil droplets owing to evaporation of a continuous water phase

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Abstract

Coating and drying of emulsions are frequently used to express the functionality of many industrial products, such as cosmetics, adhesives or ink. The use of solid particles instead of surfactant molecules has been recently attractive in terms of longer lifetime and additional functionalities of the products [1], which is named Pickering emulsion. However, fundamental knowledge of how Pickering emulsions are dried is still lacking. When an oil-in-water (O/W) type of emulsion, where involatile oil droplets are dispersed in water, is dried, the droplets are compressed, get deformed and eventually coalesce due to the evaporation of the continuous water phase. It has not been fully understood how well the droplets get deformed and coalesce during water evaporation depending on physical properties such as ion concentration or particle concentration in water. In this presentation, two topics on drying of Pickering emulsions are discussed: (i) the effect of salt concentrations in water on the coalescence of the dispersed oil droplets [2]; (ii) the coalescence of monodispersed Pickering emulsions made with microfluidic technique.

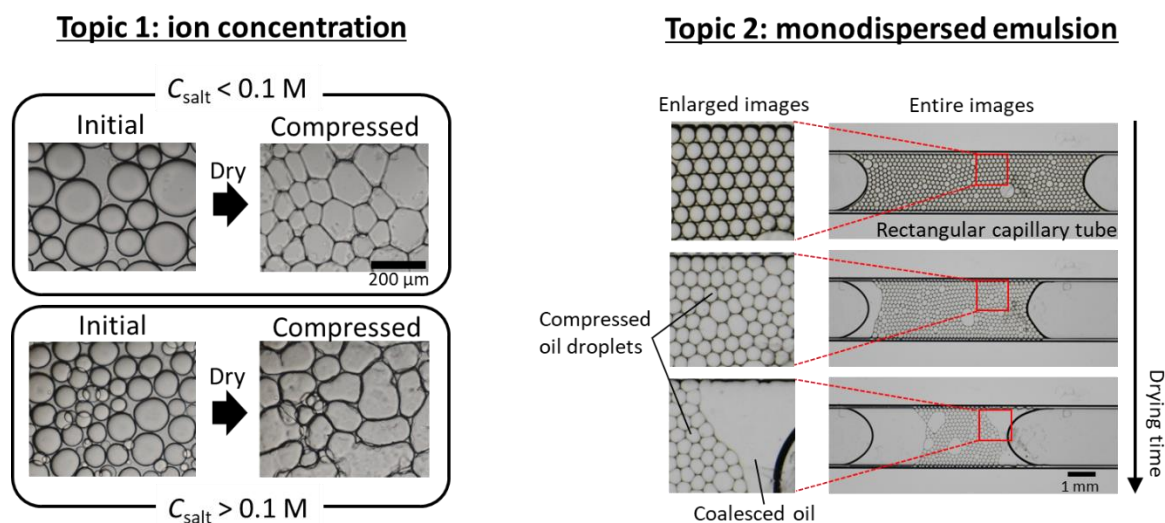


Figure 1. Two topics described in my presentation. (left) effect of ion concentrations on droplet coalescence. (right) drying of a O/W monodispersed Pickering emulsion prepared with microfluidic device

Keywords: particle-stabilized emulsion, drying, deformation, coalescence

References

- [1] B. P. Binks, P. D. I. Fletcher, A. J. Johnson, I. Marinopoulos, J. M. Crowther and M. A. Thompson, *ACS Appl. Mater. Interfaces*, **8**, 21201-21213 (2016).
- [2] K. Abe and S. Inasawa, *Colloids and Surfaces A: Physicochem. Eng. Asp.*, **632**, 127816 (2022).

Rheology study of complex fluids using mesoscale simulations and its application towards the process relevant energy storage materials

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Abstract

Complex fluids, including particulate suspensions, are encountered in a multitude of industrially relevant processes, for example, semiconductors, secondary batteries, and displays, to list a few. Understanding the factors that affect the flow characteristics of complex fluids and how to manipulate them is crucial for improving product quality. Despite the efforts of pioneers, the influences of size distributions and interactions among components on complex fluids, have not been fully understood yet. Inspired by this point, we explore the rheology of mixtures consisting of particles with significant size differences through numerical simulation. Describing the target system presents a challenge due to theoretical and technical difficulties in managing the significant differences in length and time scales among its components. To address this issue, we employ the "mesoscale simulation" technique. In this talk, we briefly introduce a strategy to achieve our study and its applications toward the development of processes for energy storage materials.

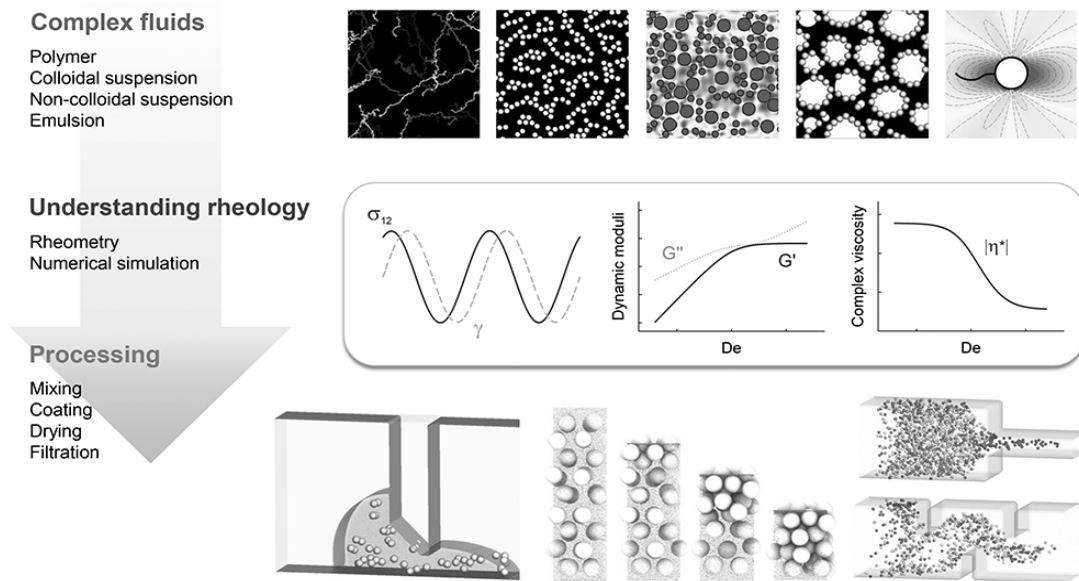


Figure 1. Schematic diagram for applying mesoscale simulation towards the process development

Keywords: Rheology, complex fluids, mesoscale simulation, processes, energy storage materials

Value Chains among University, Chemical Company, and Industrial Machine Company

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Abstract

In Japan, the birthrate is declining, the population is aging, and the working-age population has been declining significantly in recent years. The manufacturing industry, one of Japan's major export industries, is also facing a serious labor shortage, especially among small and medium-sized companies, after the Corona disaster.

On the other hand, many Japanese industrial machinery manufacturers have huge back orders for lithium-ion rechargeable battery manufacturing equipment and semiconductor manufacturing equipment, which are booming. These companies are reallocating their valuable R&D personnel to the design department to settle the backlog of orders under the customer-first policy. Although this has increased sales in the short term, the board members of company management concern that the stagnation of R&D due to reassignment causes a decline in competitiveness in the near future.

The research environment at universities has been heavily dependent on competitive funding from the Japanese government, and submitting papers to high impact factor journals and earning a large number of citations are becoming prerequisites for obtaining research funding. In addition to the fact that global competition is based on such indicators, the reasons for this situation include the fragmentation of research themes and review fatigue caused by the proliferation of competitive funds. Therefore, there is a tendency to evaluate research fairly using universal indicators that are easy to understand, even without a deep understanding of the research content. Research themes are concentrated on relatively inexpensive themes that are easy to publish, and research themes related to industrially important production technology tend to be avoided.

The Japanese government's research funds come from taxes paid by citizens and corporations, and it is necessary for Japanese university faculty members to collaborate in research and development while maintaining close relations with industry. Considering such a situation in the Japanese manufacturing industry, we have constructed a value chain as shown in Fig. 1 and are conducting R&D jointly.

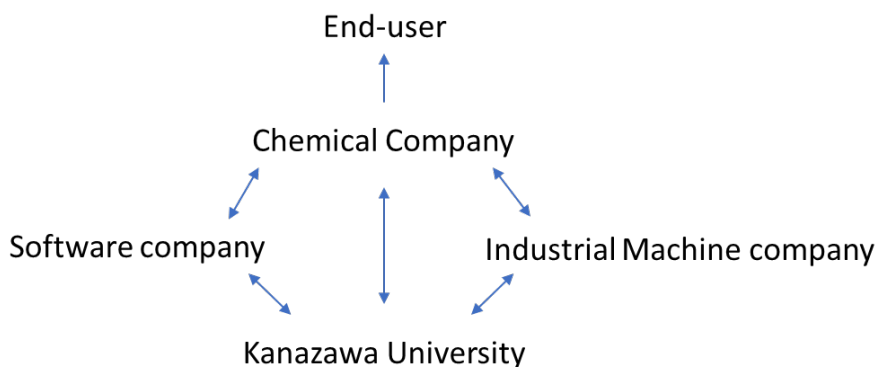


Figure 1. Value chain of chemical process, industrial machine, end end-user companies.

Keywords Value chain, process engineering, chemical engineering, precision wet-coating.

References

Location : Vision Hall (6th floor)

Time	No.	Title	Presenter
Oral session I (Session chair : Prof. Kentaro Taki)			
13:30-13:45	O-1	Airflow Analysis of a Coating Room by Full Cloud CAE	Nobuo Hamamoto (<i>AndanTEC</i>)
13:45-13:55	O-2	Evaluation of electrochemical and rheological properties of lithium ion battery anode slurries from Bench-scale in-line pipe flow	Chan Hyeok Ahn (<i>Seoul National Univ.</i>)
13:55-14:05	O-3	Fabrication of Liquid Metal Soldering Composite with Ultra-low Reflow Temperature for Surface-mount Technology of Flexible Printed Circuit Board	Fang-Chen Kuo (<i>National Taiwan Univ.</i>)
14:05-14:15	O-4	Evaluating the Role of Binders and Active Materials for Anode Slurries Using Nonlinear Rheological Properties	Jeonghyeon Lee (<i>Pusan National Univ.</i>)
14:15-14:25	O-5	Rapid UV Curing DES Coatings with Enhanced Conductivity and Antimicrobial Properties	Jia-Yu Yang (<i>National Sun Yat-sen Univ.</i>)
14:25-14:35	Coffee break		
Oral session II (Session chair : Prof. Dongjae Kim)			
14:35-14:45	O-6	Addressing Instability in Interface Tracking of Transient Computation of Free-Surface Flow	Yundong Yang (<i>Seoul National Univ.</i>)
14:45-14:55	O-7	A Predictive Model Enabling Ultrahigh Particle Containing Composite for High-Performance Packaging Materials	Wei-Cheng Chao (<i>National Taiwan Univ.</i>)
14:55-15:05	O-8	Visualization of extensional flow of complex fluids through DoS-CaBER and analysis through Machine learning	Minhyuk Im (<i>Seoul National Univ.</i>)
15:05-15:15	O-9	Refining Bacterial Cellulose Packaging with Mercerization, In-Situ Spraying, and Dip Coating Techniques	Cheng-Ying LI (<i>National Taiwan Univ.</i>)
15:15-15:25	O-10	The Synthesis of AgNPs/skim natural rubber/bacteria cellulose bio- polymeric composite for humidity sensor	Puttakhun Meemai (<i>National Taiwan Univ.</i>)
15:25-15:35	Coffee break		
Oral session III (Session chair : Prof. Yi-Ju Chou)			
15:35-15:45	O-11	Trends of vortex formation in the feed slot of slot coating flows	Sangho Oh (<i>Seoul National Univ.</i>)
15:45-15:55	O-12	What governs kinetics of water evaporation from polymer solutions?	Masahiko Tanaka (<i>Tokyo Univ. of Agriculture and Technology</i>)
15:55-16:05	O-13	Thermally Conductive Polymer Composite for Thermal Management Material	Yi-Chen Weng (<i>National Taiwan Univ.</i>)
16:05-16:15	O-14	How the molecular weight of carboxymethyl cellulose affects the dispersion of silicon particles for lithium-ion batteries	Kyeong Jin Kim (<i>Seoul National Univ.</i>)

Airflow Analysis of a Coating Room by Full Cloud CAE

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Abstract

Airflow control in Roll To Roll process is definitely important to create optical film to avoid layer surface unevenness caused by dry air disturbance. Furthermore, inflow air from the circumstance zone should be excluded to lessen the defect as well.

Nevertheless the importance of the invisible airflow in the coating room is hardly comprehended, so each process operators set the condition experientially.

Aside from these difficulties, airflow analysis technology dramatically evolves, recently. The progress makes it possible to analyze the detailed airflow in the coating area in 3D. The study is based on a full-cloud CAE platform developed by SimScale which is suitable for this kind of simulation.

The application tool requires only CAD info upload, then setting a condition, executing calculations, and visualizing automatically on the cloud. Plus simultaneous multiple execution saves calculation time. The simulated result is shown below.

- (1) down flow from the ceiling directly disturbs the surface layer just after coating,
- (2) a slight pressure difference of 1(pa) level causes air inflow from before/after zone of the coating room,
- (3) the narrower slits gap of film in/outlet to the coating room, the lessen the air inflow from before/after zone.

This kind of analysis is not only effective for productivity but worthwhile for the designing process.

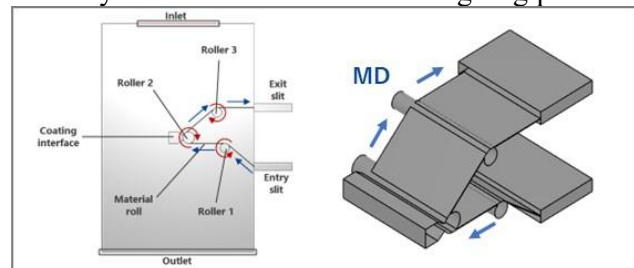
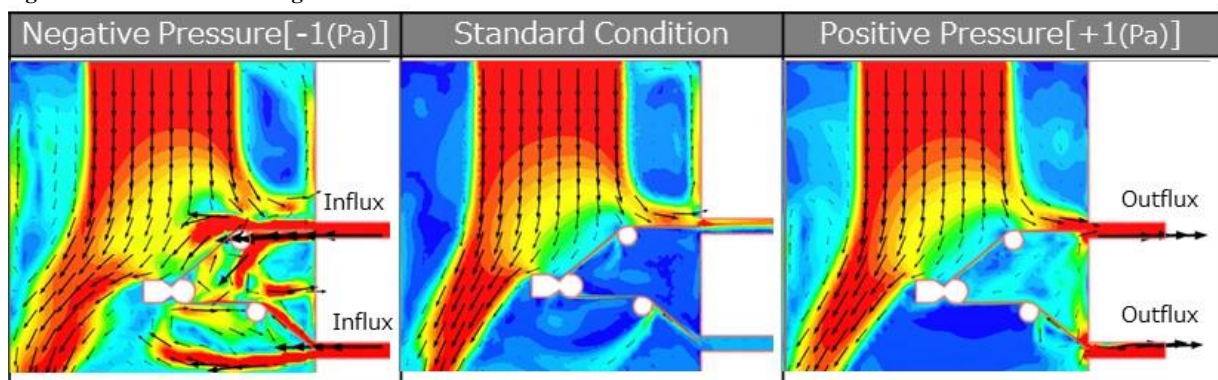


Figure 1. Layout of Coating Room

Figure 1. Airflow in a coating room



Keywords: CAE, FVM, Coating, Clean Room, Roll To Roll, Airflow

References

- [1] Hamamoto, N., JP4881750 (2007)
- [2] Hamamoto, N., Convertec, pp38-44(2022.4)

Evaluation of electrochemical and rheological properties of lithium ion battery anode slurries from Bench-scale in-line pipe flow

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Abstract

Today, many suspensions are characterized by a high solid content to achieve enhanced functionality, and lithium ion battery electrode slurry is a representative example of high solid content suspension(slurry). Effectively managing slurry with excellent dispersibility in large-scale processes is crucial for ensuring stability and optimal performance. However, the flow properties of the electrode slurries are hard to define clearly due to its complex and unclear rheological and micro-structural properties which are subject to potential changes by compositional and process conditions (variance by flow time, filtration, local compositional changes). Therefore, comprehensive evaluation through various means, incorporating environmental variables, is necessary.

In this research, we evaluated the carbon-based anode slurry under pipe flow conditions with long time-scale. Bench-scale anode slurries that have different compositions and dispersion properties were made for the evaluation. The rheological evaluation was conducted by slurry sampling during the pipe flow. Also, continuous datasets from pressure, guide-wave velocimetry, and electrochemical impedance spectroscopy (EIS) were analyzed. Series of experiments showed that the small amount of difference in polymer dispersant content can cause significant differences both in the rheological and electrochemical properties, even if the sufficient amount of polymer dispersant exist. Also, the massive continuous datasets of pressure, collected during the flow process, were normalized, and the machine-learning was applied for the classification.^[1] We successfully classified the slurries in two ways: one method distinguished temporal changes during the flow, while the other method successfully differentiated the slurries with different compositions.

Keywords: in-line pipe flow, lithium-battery anode slurry, EIS, machine-learning, in-line evaluation

References (10 Bold)

- [1] Kang, Seunghoon, et al. "Classification of battery slurry by flow signal processing via echo state network model." *Rheologica Acta* 62.10 (2023): 605-615.

Fabrication of Liquid Metal Soldering Composite with Ultra-low Reflow Temperature for Surface-mount Technology of Flexible Printed Circuit Board

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Abstract

With the growing demand for highly compatible wearable devices, the requirement for flexible printed circuit board (FPCB) keeps increasing. However, the high reflow-temperature of conventional soldering process would cause heat damage to the soft polymer substrates due to their low phase-transition temperatures, including glass-transition temperature and melting point. Liquid metals (LM) were then proposed as substitutes for conventional soldering alloys because of their fluidity under low temperature, which also causes some issues, including leaking and low mechanical property. To solve the problem, amalgamation-inspired method was introduced to this study for solidification and mechanical property enhancement of LM solders.

In this study, GaInSn/Cu soldering composite is prepared by simply mixing Cu powders with LM alloy (GaInSn) until they are completely wetted by GaInSn. Amalgamation-inspired solidification reaction of the GaInSn/Cu soldering composite, including formation of CuGa_2 intermetallic compounds (IMC) and In-Sn-Ga solid solution, happens spontaneously. Furthermore, an isothermal heating process at only 70°C is able to accelerate the solidification reaction. DSC analysis reveals that the melting point of GaInSn/Cu soldering composite increases from around 61.4°C (below the operating temperature of 70°C) to about 106°C after the isothermal heating process. This confirms that the procedure in this study successfully triggers the solidification reaction, which solves the leaking issue of solder joints. Also, the composition change within GaInSn/Cu composite is verified by XRD analysis. To address the issues of low mechanical strength and prolonged solidification time in solder joints made from liquid solder, this study references the Ga-In-Sn ternary phase diagram to adjust the composition of GaInSn/Cu soldering composite. The results of lapping shear strength of solidified solder joints indicate that the shear strength reached approximately 51.3 MPa, being 100 times higher than the values before composition adjustment, and roughly 5 times higher than in other related studies [1]. The GaInSn/Cu soldering composite and amalgamation-inspired soldering process in this study require low reflow temperature of only 60°C, preventing heat damage to FPCB substrates and advancing the surface-mount technology of FPCB.

Keywords: Flexible printed board, Surface-mount technology, Low-temperature soldering paste, Liquid metal

References

- [1] Zheng, Zenghuang, et al. "Low - Temperature Solidifiable Liquid Metal with Ultrahigh Thermal Conductivity Enabled by Spontaneous Phase Transition for Electronics' Safety and Long - Life Cooling." *Advanced Engineering Materials* 25.11 (2023): 2201817.

Evaluating the Role of Binders and Active Materials for Anode Slurries Using Nonlinear Rheological Properties

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Abstract

The fluidity and stability of lithium-ion electrode slurries are critical in high-speed, high-temperature, and high-pressure manufacturing processes. Poor-quality slurries can clog pipes during transportation or degrade adhesion in the coating process, causing cracks in the electrodes. Anode slurries are composed of conductive additives, active materials, binders, and solvents, all of which affect particle dispersion and microstructure [1]. Many studies have been conducted on the linear viscoelastic behavior of electrode slurries to understand the particle dispersion and microstructure of the slurry, but it has not been noted that during the electrode production process, the slurry is exposed to very high shear rates and large deformations. Therefore, the study of the nonlinear rheological behavior of electrode slurries can provide a comprehensive insight into the microstructural changes of slurries subjected to large deformations in real industry.

This study covers several rheological properties of anode slurries but focuses on the effects of different molecular weights of binders and different types of active materials on the nonlinear rheological properties of anode slurries. The materials used in the study are carbon black (CB) as a conductive additive, two types of graphite (Gr, flake and spherical) as an active material, carboxymethyl cellulose (CMC, Mw=90, 250, 700 kg/mol) with three different molecular weights as a binder, and finally water as a solvent.

First, optical microscopy (OM) was used to image the dispersion of the particles in the slurry. However, the slurry has a very high particle content, and the slurry must be diluted in order to observe the dispersion of the particles. This means that the images used in the analysis do not accurately reflect the actual microstructure of the slurry, so an additional rheological approach is needed to better understand the microstructure formation and deformation of the slurry.

To identify and quantify the thixotropy of the anode slurry as a function of binder and active material, the rheological hysteresis loop area was calculated. Additionally, large amplitude oscillatory shear (LAOS) tests performed to measure the nonlinear rheological properties allowed us to observe and classify different LAOS types [2], such as two-step strain thinning and strain overshoot. We also calculated the intrinsic nonlinearity coefficient (Q_0) [3] and nonlinear-linear viscoelastic ratio (NLR) values [4] for different anode slurries using the Fourier transform (FT)-Rheology. By using NLR values that normalized the graphite-containing slurry to a graphite-free CMC/CB suspension, the degree of dispersion of graphite in the slurry could be quantified and compared.

Furthermore, the surface of the films prepared by coating and drying the slurry was observed using field emission scanning electron microscopy (FE-SEM) to confirm that the positional relationship formed between carbon black and graphite varies depending on the type of graphite.

Keywords : Electrode rheology, Anode slurry, LAOS, NLR, Thixotropy, Rheological hysteresis

References

- [1] S Lim, S Kim, KH Ahn, SJ Lee, *The effect of binders on the rheological properties and the microstructure formation of lithium-ion battery anode slurries*. Journal of Power Sources, 299, 221-230 (2015)
- [2] K Hyun, SH Kim, KH Ahn, SJ Lee, *Large amplitude oscillatory shear as a way to classify the complex fluids*. Journal of Non-Newtonian Fluid Mechanics, 107(1-3), 51-65 (2002).
- [3] K Hyun, M Wilhelm, *Establishing a New Mechanical Nonlinear Coefficient Q from FT-Rheology: First Investigation of Entangled Linear and Comb Polymer Model Systems*. Macromolecules, 42(1), 411-422 (2009).
- [4] HT. Lim, KH. Ahn, JS. Hong, K Hyun, *Nonlinear viscoelasticity of polymer nanocomposites under large amplitude oscillatory shear flow*. J. Rheol. 57 (3), 767-789 (2013).

Rapid UV Curing DES Coatings with Enhanced Conductivity and Antimicrobial Properties

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Abstract

In this study, we present a breakthrough in coating technology with the development of multifunctional coatings using deep eutectic solvents (DES) as a novel alternative to traditional water-based solutions. By blending different DESs, we have formulated coatings with customizable mechanical and conductive properties, outperforming conventional hydrogel coatings. A standout feature of these DES-based coatings is their ability to rapidly cure under UV exposure, achieving full solidification in just 10 seconds. This rapid curing capability greatly enhances the efficiency of the coating process, making it highly suitable for industrial applications.

These coatings demonstrate exceptional mechanical strength, high transparency of 94%, biocompatibility, and antimicrobial properties against agents like *E. coli*, making them ideal for a wide range of applications, including in the fields of flexible electronics, soft robotics, and healthcare. The coatings maintain their performance under extreme temperatures (-70°C to 80°C) and have been extensively tested for environmental stability.

Furthermore, the DES ionic gel exhibits a broad strain sensing range (1% to 400%) and can operate effectively within a temperature range of 15°C to 50°C, showcasing its adaptability to various environmental conditions. Their application in monitoring human activities and vital signs has been successfully demonstrated, indicating their potential in bio-integrated devices and healthcare applications.

This research provides significant insights into the development of advanced coating materials, particularly highlighting the rapid UV curing property, which is crucial for applications demanding quick and efficient coating processes. Our findings mark a significant advancement in coating technologies, paving the way for future innovations in environmentally stable, biocompatible, and efficient coating solutions.

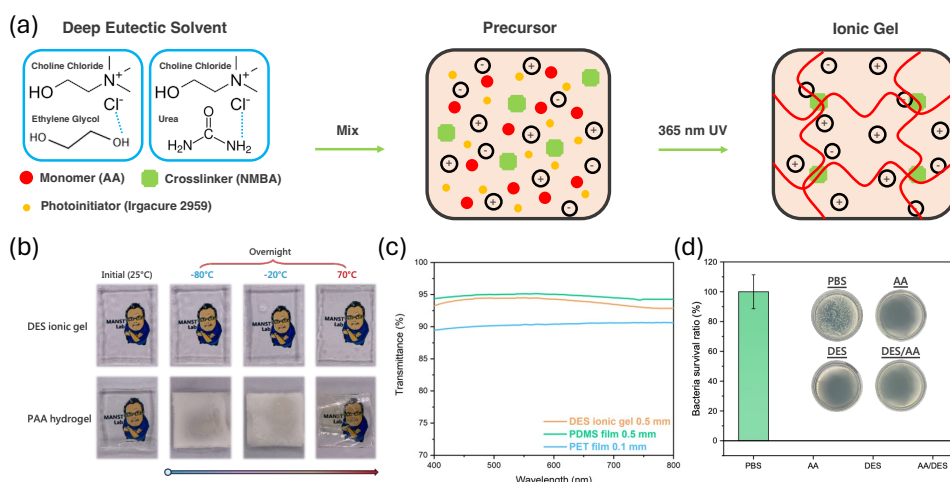


Figure 1. (a) Schematic diagram of DES ionic gel preparation; (b) environmental stability; (c) transparency; (d) antibacterial properties

Keywords: UV curable, deep eutectic solvents, ionic gel, biocompatible, antibacterial, sensors

References

- [1] Ma, Y.; Zhang, Y.; Cai, S.; Han, Z.; Liu, X.; Wang, F.; Cao, Y.; Wang, Z.; Li, H.; Chen, Y.; Feng, X. Flexible Hybrid Electronics for Digital Healthcare. *Advanced Materials* 2020, 32 (15), 1902062. <https://doi.org/10.1002/adma.201902062>.
- [2] Park, S.; Heo, S. W.; Lee, W.; Inoue, D.; Jiang, Z.; Yu, K.; Jinno, H.; Hashizume, D.; Sekino, M.; Yokota, T.; Fukuda, K.; Tajima, K.; Someya, T. Self-Powered Ultra-Flexible Electronics via Nano-Grating-Patterned Organic Photovoltaics. *Nature* 2018, 561 (7724), 516–521. <https://doi.org/10.1038/s41586-018-0536-x>.

Addressing Instability in Interface Tracking of Transient Computation of Free-Surface Flow

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Abstract

Understanding the behavior of interfaces in engineering processes involving fluids is crucial, particularly in industries like secondary battery manufacturing that utilize coating processes. These processes often involve numerical computations to replicate interfaces, such as liquid-gas interfaces with high aspect ratios and shear rates. However, challenges arise due to the instability of these interfaces caused by oscillatory solutions along the material's length. This instability is due to the reflective behavior induced by the arbitrarily truncated free surface involving an artificial outflow.

The study focuses on the instability caused by boundary conditions, especially the free surface's kinematic condition for the nodal displacements. These conditions lead to fluctuations in the pressure field and wiggles in the interface [1]. One option for the kinematic condition is Nitsche's method, which weakly imposes nodal displacements on the free surface [2]. The study proposes modifying Nitsche's method, which weakly imposes only the normal direction with a penalty term. This method aims to alleviate excessive impositions while maintaining stability in interface computations by comparing the transient behavior of the L2-norm error in solution with the previous timestep.

By applying this practical and applicable modified method to a 2-D model problem representing the shear flow in the coating process, the study investigates the impact of relaxing imposition on transient behavior and interface instability. This study used the in-house finite element method software to conduct a numerical method based on the interface tracking method. The findings of this study could provide valuable insights into stable interface simulations in various real-world engineering processes involving liquid-gas interfaces.

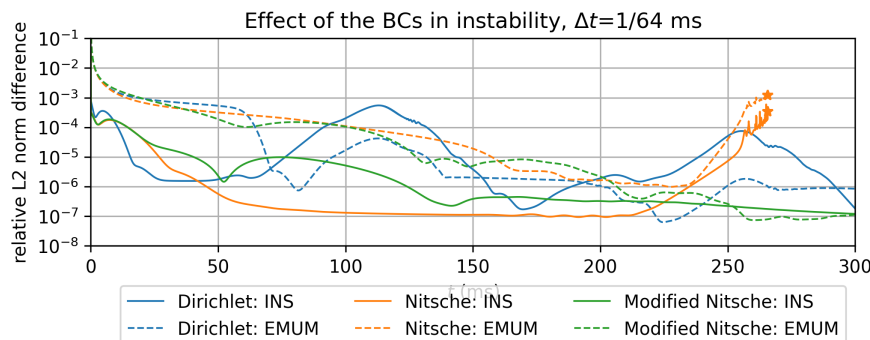


Figure 1. Transient solutions exhibit spurious instabilities that depend on the boundary conditions (BCs). INS represents the flow field data, while EMUM represents the nodal displacement field data.

Keywords: Computational fluid dynamics, Finite element method, Interface tracking, Nitsche's method

References

- [1] Sani, R. L., Gresho, P. M., Lee, R. L., & Griffiths, D. F. (1981). *The cause and cure (?) of the spurious pressures generated by certain FEM solutions of the incompressible Navier-Stokes equations: Part 1*. Int. J. Numer. Methods Fluids, 1(1), 17-43.
- [2] Lu, K., Augarde, C. E., Coombs, W. M., & Hu, Z. (2019). *Weak impositions of Dirichlet boundary conditions in solid mechanics: a critique of current approaches and extension to partially prescribed boundaries*. Comput. Methods Appl. Mech. Eng., 348, 632-659.

A Predictive Model Enabling Ultrahigh Particle Containing Composite for High-Performance Packaging Materials

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Abstract

With the rapid advance of semiconductor manufacturing, the demand for better-performance packing materials that prevent chips from damping, oxidation, and contamination grows enormously. Therefore, the requirement for properties including higher thermal conductivity [1], lower thermal expansion coefficient (CTE, α_1 and α_2) and Dk/Df values are rising [2]. Liquid epoxy molding compounds (LMCs) composed of epoxy resin, ceramic particles, and additives are currently the most advantageous materials for flip-out wafer-level packaging (FOWLP). Previous literature shows that increasing the solid content of ceramic particles, usually silica, inside the LMC can effectively elaborate its physical properties so that approaches the requirement above. However, the increasing solid content inevitably leads to viscosity increment and processibility reduction issues which limit the solid content to 80 weight percentage (wt%) for LMCs.

In this study, an empirical model is developed based on the Krieger-Dougherty equation and the Sudduth model to directly correlate the particle size distribution of dispersed particles with the zero-shear viscosity of so-made liquid composites. The model is applied to determine the blending ratio and size ratio between distinct size distribution silica particle samples for reaching the optimal maximum packing density of particles inside the solvent. The established model forecasts the achievement of an optimal packing density of 0.97 by incorporating particle samples with a size ratio of 0.1 in a 7 to 3 volume ratio, and the fitting results by the Krieger-Dougherty equation further verify the prediction precision of our model. Furthermore, the generality and accuracy of the model are evidenced by the exceptionally precise prediction of the zero-shear viscosity of composites containing an arbitrarily selected combination of silica samples. For liquid encapsulation application, 78 vol% silica/epoxy composite enabled by the model is made into the ultrahigh solid-content LMC, which possesses a thermal conductivity as high as 1.33 W/mK, close to that of pure silica particles. Also, both the achievement of low α_1 and α_2 (13.2 and 23.3 ppm/°C respectively) and high glass transition temperature (142.4 °C) emphasize the excellent contribution of the model for reaching composites with ultrahigh particle addition. Last but not least, 78 vol% LMC can successfully coat onto a 4-inch wafer with controllable thickness and complete covering while maintaining low surface roughness ($R_q < 0.3 \mu\text{m}$) compatible with the PET film. The exhibition of Dk/Df values of 2.62/0.00618 are significantly lower than FR-4. In conclusion, the outstanding physical properties achieved by the ultrahigh solid-content LMCs demonstrate the remarkable performance of the established model, which possesses great practicality for industrial application.

Keywords: particle composite, viscosity, maximum packing density, liquid epoxy molding compounds, liquid encapsulation

References

- [1] X. Huang, P. Jiang, T. Tanaka, A review of dielectric polymer composites with high thermal conductivity, IEEE Electr. Insul. Mag. 27(4) (2011) 8-16.
- [2] Z.Q. Zhang, C.P. Wong, Recent advances in flip-chip underfill: Materials, process, and reliability, IEEE Trans. Adv. Packaging 27(3) (2004) 515-524. <https://doi.org/10.1109/Tadvp.2004.831870>.

Visualization of extensional flow of complex fluids through DoS-CaBER and analysis through Machine learning

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Abstract

Understanding and analyzing capillary-driven extensional flow dynamics is crucial for applications like inkjet printing and emulsion formation. However, the spatio-temporal shapes of complex fluids as they stretch have been partially analyzed by conventional methods that measure only single points in the slender jet approximation, even though their shapes contain important rheological information.

We introduce a novel approach that integrates machine learning and flow visualization to classify and estimate fluid composition without relying on traditional rheological models. Our method utilizes captured images using dripping onto substrate capillary break-up extensional rheometry (DoS-CaBER)[1], which specializes in observing the spatio-temporal dynamics of capillary-driven extensional flows. Through these images, we introduce *eigen-thinning* extracted via principal component analysis (PCA), enabling fluid classification and composition estimation. A *k*-nearest neighbor (*k*NN) classification achieves nearly 100 % accuracy using a few Principal Components (PCs). We extend this to multi-component fluid composition estimation with promising results.

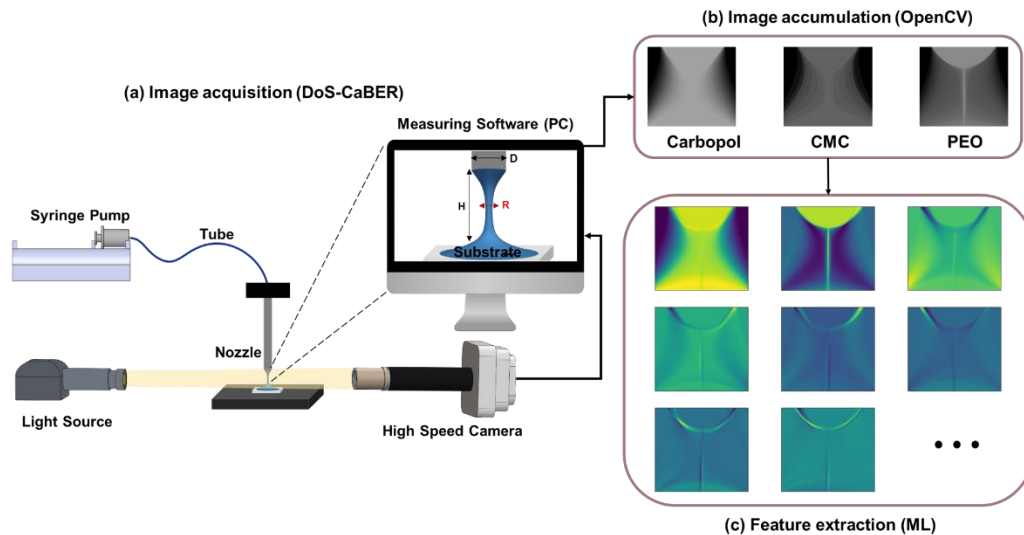


Figure 1. Schematic diagram of extensional flow visualization and analysis processes.

Keywords : Capillary-driven extensional flow, Dripping onto substrate capillary break up extensional rheometry(DoS-CaBER), Principal component analysis, Machine learning, Complex fluid dynamics

References

[1] Vivek Sharma et al., Proceedings of the National Academy of Sciences. 116.18, 8766-8774 (2019).

Refining Bacterial Cellulose Packaging with Mercerization, In-Situ Spraying, and Dip Coating Techniques

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Abstract

With the increasing demand for packaging applications, the necessity to replace petrochemical products has become more evident than ever [1]. Bacterial cellulose (BC), renowned for its remarkable physical properties and sustainability, stands as one of the potential alternatives. However, challenges such as low ductility, limited transparency, absence of antibacterial properties, and weak barrier properties hinder its application in packaging. In this study, we employed an in-situ spraying method to produce antimicrobial bacterial cellulose, enabling the uniform encapsulation of antimicrobial properties in an economically and environmentally friendly manner. With a mercerization treatment, ductility increased by fivefold, while haze decreased by 50%. The swelling ratio exhibited only 10% of the deviation compared to the original. After dip coating with waterborne polyurethane (WPU), a multi-layered composite film was fabricated. Consequently, the composite film demonstrated commendable water vapor and oxygen barrier properties similar to those of commercial plastic film. Furthermore, transparency was further improved due to hole filling in the structure and reduced surface roughness. The BC/CS/WPU composite film demonstrated notable effectiveness in preserving egg freshness, as evidenced by the absence of bacterial growth on the eggs in comparison to both control and commercial alternatives. This study introduces promising methodologies for augmenting the ductility, transparency, antibacterial attributes, and barrier functionalities of bacterial cellulose. These strategies may also hold potential for application in diverse polysaccharide modifications to replace non-biodegradable plastics.

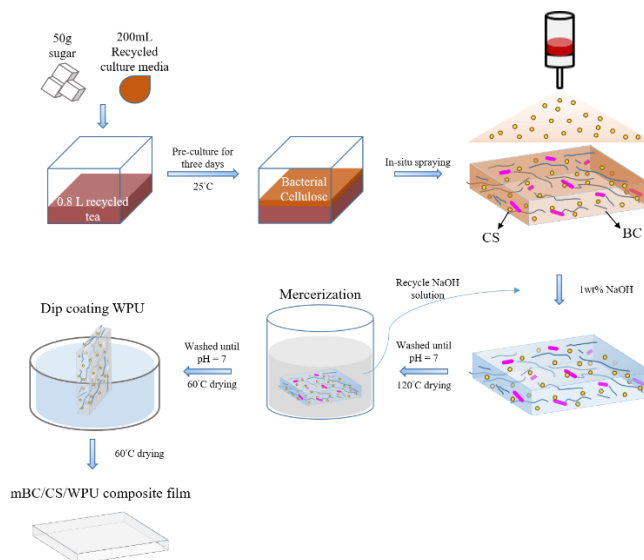


Figure 1. Schematic diagram of BC/CS/WPU synthesis process.

Keywords: Bacterial cellulose, packaging, mercerization, in-situ spraying, and antimicrobial properties

References

1. Xia, J., et al., *Multifunctional sustainable films of bacterial cellulose nanocrystal-based, three-phase pickering nanoemulsions: A promising active food packaging for cheese*. Chemical Engineering Journal, 2023. **466**: p. 143295.

ACW2024 (May 8-10, 2024), LG Science Park, Seoul, Korea

The Synthesis of AgNPs/skim natural rubber/bacteria cellulose bio- polymeric composite for humidity sensor

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Abstract

The rapid growth of electronic waste (e-waste) poses a global environmental and health challenge due to hazardous solvents in processing. Utilizing bio-polymeric composite derived from renewable sources offers a promising solution. These sustainable alternatives can reduce reliance on non-renewable resources, minimize environmental footprints, and provide safer end-of-life disposal options. Introducing bio-polymers in electronics manufacturing represents a significant step towards a more sustainable and circular economy, ensuring that electronic waste is effectively managed, and environmental impacts are minimized.

In this research, a green synthesis method was developed to produce bio-polymeric conductive composites. Bacterial cellulose (BC) was modified through the integration of silver nanoparticles (AgNps) in skim natural rubber latex (SNR). First, AgNps were directly synthesized by using silver nitrate (AgNO₃) solution of 40-160 mM adding in SNR suspension under a reduction reaction at 50 to 80 °C. Secondly, to enhance electrical conductivity and mechanical properties, pure bacterial cellulose pellicle was immersed into the prepared AgNps-SNR suspension for 48 h before washing and drying, respectively. The composite films of AgNps/SNR/BC were then investigated for chemical, physical, antibacterial properties, and electrical. The AgNps/SNR/BC films demonstrated potent antibacterial activity against *Staphylococcus aureus* and *Escherichia coli*, attributed to the incorporation of AgNps. Additionally, the strain at break of the composite films was significantly enhanced up to 13.8 % under the treatment using 80 mM AgNO₃ and 80 °C. Furthermore, the incorporation of AgNps significantly improved the electrical conductivity of composite films. AgNps/SNR/BC films treated with 80 mM of AgNO₃ exhibited the highest electrical conductivity at 4.09×10^{-7} S/cm. Given these improved properties, the developed composite films hold promising potential for applications in humidity sensing. Accordingly, the composite films, 80Ag-SNB-80 exhibit excellent response times/ recovery time (~ 3/20 s) with a wide humidity-sensing range from 30% RH to 90% RH. Overall, this study demonstrates the excellent conductivity and mechanical properties of the biopolymer AgNps/SNR/BC composite, providing applications in humidity sensors.

Keywords: Bio-based polymer, Silver nanoparticles, Skim natural rubber, Bacteria cellulose, Conductivity properties, Humidity sensor

Trends of vortex formation in the feed slot of slot coating flows

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Abstract

Slot coating is a key method used in coating battery slurry electrodes to achieve a uniform and stable end product. It is crucial to prevent defects during this process, with vortex formation in the feed slot being a particularly critical issue. Vortices in the feed slot can lead to uneven flows and particle coagulation, resulting in defects in the final product.

This study focuses on quantifying and analyzing the vortices generated in the feed slot during slot coating under different process conditions. Geometry and process parameters were varied. By comparing Newtonian and Carreau fluids, the impact of shear-thinning characteristics on vortex formation was also investigated. Computational simulations using the Finite Element Method and clustering techniques for vortex quantification were employed.

The analysis revealed that increasing the feed slot height promotes vortex generation compared to the coating gap. Higher substrate speeds relative to the flow rate were found to enhance vortex formation. Additionally, shear-thinning characteristics were shown to inhibit vortex formation. These findings offer valuable insights for optimizing the coating process and addressing vortex-related issues.

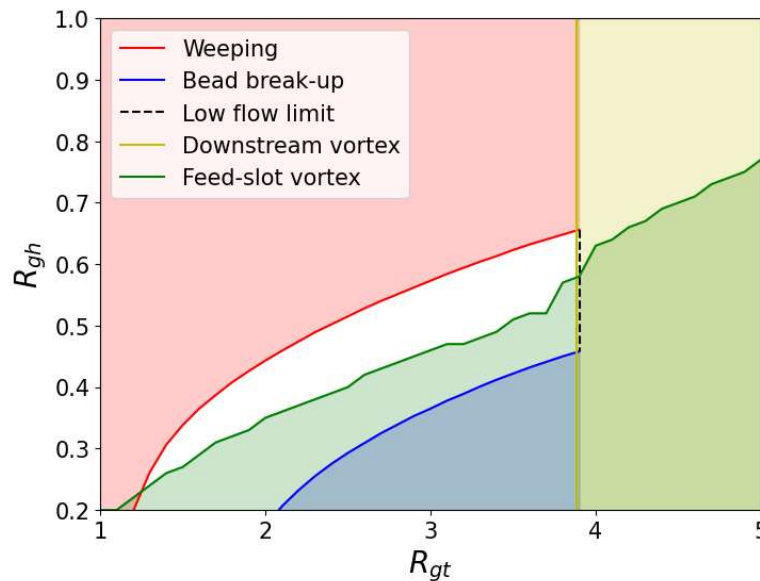


Figure 1. The operability window with the vortex map for the Carreau fluid

Keywords: Slot coating, Vortex, Feed-slot, Shear thinning, Finite element method, Clustering

References

- [1] Sartor, L. Slot Coating: Fluid Mechanics and Die Design. (1990).
- [2] Nam, J., Scriven, L. E. & Carvalho, M. S. Tracking birth of vortex in flows. *J Comput Phys* 228, 4549–4567 (2009).
- [3] Kwak, H. & Nam, J. Simple criterion for vortex formation in the channel flow of power-law fluids. *J Non-newton Fluid* 284, 104372 (2020).
- [4] Kwak, H. & Nam, J. Simple methods for obtaining flow reversal conditions in Couette–Poiseuille flows. *J Rheol* 65, 1023–1033 (2021).

What governs kinetics of water evaporation from polymer solutions?

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Abstract

Solvent evaporation from a polymer solution is a key process to produce polymer films. Polymer molecules accumulate near the evaporating interface as drying proceeds, and they form a concentrated polymer layer called as a skin layer. This layer is generally considered as a barrier for solvent evaporation. Drying kinetics of polymer solutions is a basic to design the film formation process, but it is also a very important clue to understand properties of water in concentrated solutions, such as water chemical activity^[1]. In this talk, we will show how the polymer type and size (molecular weight) affect drying rates of aqueous polymer solutions. Fig. 1 shows an example of drying rates of sample solutions with different initial polymer concentrations (C_0). Drying rates are well summarized with the amount of polymer transported to the evaporating interface (integral in x axis of Fig. 1 (b)), and it is independent of C_0 . We will discuss what property of polymer (solution) affects the drying kinetics of water.

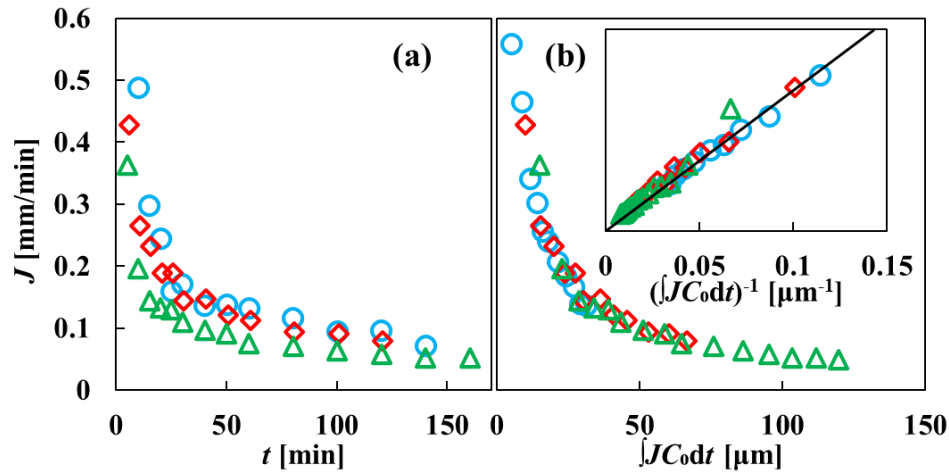


Figure 1 (a) Time lapses of drying rates (J s) of aqueous polyvinyl alcohol solutions. (b) The same data in (a) but replotted with the term of $\int_0^t JC_0 dt$ (inset: $(\int_0^t JC_0 dt)^{-1}$), that corresponds to the transported amount of polymer to the evaporating interface. The solid line in the inset in (b) shows $y = 4.3x$. Initial polymer concentrations (C_0 s) are ○ 0.2 vol%, ◇ 0.4 vol% and △ 0.8 vol%, respectively.

Keywords: Water evaporation, aqueous polymer solution, polymer accumulation, polymer size/type

References

[1] J.B. Salmon et al., *Phys. Rev. E*, 96 (2017), 032612

Thermally Conductive Polymer Composite for Thermal Management Material

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Abstract

With the development of wearable devices, the increasing demand for the miniaturization and integration of electronic components has highlighted the importance of heat dissipation. Effective heat dissipation is crucial for maintaining the stability and lifetime of high-energy-density electronic devices [1]. Polymer is one of the materials used for heat dissipation components due to its light weight, easy processing, chemical and thermal stability, excellent electrical insulation, and low dielectric properties. Particularly, polydimethylsiloxane (PDMS) has emerged as a preferred material for thermal management in wearable devices and biomedical tissue engineering, offering the aforementioned advantages as well as its flexibility, compressibility and biocompatibility.

The incorporation of thermally conductive fillers to form composite materials is necessary due to the inherently low thermal conductivity of polymers. The thermally conductive performance of polymer composites is influenced by the filler type, shape, as well as the concentration and dispersion of the filler within the polymer matrix [2]. At low filler concentrations, better filler dispersion is helpful to increase the thermal conductivity of the composite. A higher filler concentration allows fillers to form effective thermal conduction pathways, greatly enhancing the thermal conductivity of the composite; however, it also increases the viscosity of the mixture, raising the difficulty of filler dispersion and subsequent processing.

In this study, thermally conductive composites were prepared by blending polymer and thermally conductive spherical and platelet powders respectively with the aid of three roll mill. Three roll mill can help disperse powders in the polymer uniformly and decrease the mixture viscosity. The thermal conductivity of each composite was evaluated, and the effects of filler shape and concentration on thermal conductivity were also investigated. Finally, by applying the prepared polymer composites in heat dissipation components, this study demonstrates the feasibility and potential of thermally conductive polymer composite for thermal management material.

Keywords: Polymer composite; Thermal management; Thermal conductivity; Polydimethylsiloxane

References

- [1] Y. Wen, C. Chen, Y. Ye, Z. Xue, H. Liu, X. Zhou, Y. Zhang, D. Li, X. Xie, Y.-W. Mai, *Advances on Thermally Conductive Epoxy-Based Composites as Electronic Packaging Underfill Materials—A Review*. *Adv. Mater.*, 34, 2201023 (2022).
- [2] Z. Wang, Z. Wu, L. Weng, S. Ge, D. Jiang, M. Huang, D. M. Mulvihill, Q. Chen, Z. Guo, A. Jazzar, X. He, X. Zhang, B.B. Xu, *A Roadmap Review of Thermally Conductive Polymer Composites: Critical Factors, Progress, and Prospects*. *Adv. Funct. Mater.*, 33, 2301549 (2023).

How the molecular weight of carboxymethyl cellulose affects the dispersion of silicon particles for lithium-ion batteries

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Abstract

Silicon has emerged as a promising anode material for advanced lithium-ion batteries due to its ability to significantly enhance energy density. However, silicon-containing electrodes suffer from severe instability issues due to the large volume change of silicon (~300%) during cycling, and the agglomeration of silicon particles significantly deteriorates the cyclic stability of the cell [1]. Thus, achieving homogeneous dispersion of silicon particles is essential for improving the cyclic stability of the electrodes. In this study, we investigate the influence of carboxymethyl cellulose (CMC) (degree of substitution; DS 0.7) on the dispersion of silicon particles and electrode properties, specifically focusing on the contribution of its molecular weight. We systematically adjusted the chain lengths of CMC, ranging from approximately 280kDa to 63kDa, using the ultrasonic degradation method [2]. We examine the dispersion properties of silicon particles through Si/CMC model suspensions with different molecular weights of CMC. Furthermore, we explore how changing the length of CMC chains affects the silicon dispersion in graphite/Si-blended anodes and the corresponding electrical and mechanical properties.

Keywords: Silicon, Dispersion, Agglomeration, Molecular weight, Lithium-ion battery

References

- [1] Jeschull, F., Surace, Y., Zurcher, S., Spahr, M. E., Novak, P., Trabesinger, S., *Electrochemistry and morphology of graphite negative electrodes containing silicon as capacity-enhancing electrode additive*. *Electrochimica Acta* 320, 10, 134602 (2019)
- [2] Kim, K. J., Ahn, K. H., *The effect of molecular weight of carboxymethyl cellulose on the dispersion of silicon suspensions investigated by the ultrasonic degradation method*. *Journal of the Society of Rheology, Japan* 52, 1, 1-13 (2024)

Location : Lobby of Conference Hall (5th floor)

Time	No.	Title	Presenter
16:15-17:45 (90min)	P-1	Study on the dispersion state s of carbon particles and ionomer in water/alcohol solvents using time domain NMR	Akira Ogawa (Kobe Univ.)
	P-2	Evaluation of dual-curing initiators by real-time FT-IR	Ayase Yokota (Kanazawa Univ.)
	P-3	Utilizing a data driven model for numerical simulation of non-isothermal polymer melt flow	Byeong Uk Youn (Dankook Univ.)
	P-4	Investigation of hydrodynamic for viscoelastic fluid using Lattice Boltzmann Method	Gwan Hee Jeong (Seoul National Univ.)
	P-5	Dispersion process of silica particles in epoxy resin using a planetary centrifugal mixer based on energy balance equation	Haruki Morishita (Kobe Univ.)
	P-6	Influence of hydrodynamic interaction on stratification during film drying process: Effects of particle size ratio	Heechan Kim (Korea Univ.)
	P-7	How to accurately measure the maximum adhesion force of a liquid on a solid surface	Hsi Hsuan Huang (National Taiwan Univ.)
	P-8	Assessing the impact of slurry mixing conditions on Electrochemical Lithium Recovery (ELR) system performance	Hwan Gyu Song (Dankook Univ.)
	P-9	Investigation of Flow Field Variation in Multilayer Slot Coating	Jen-Yu Hu (National Taiwan Univ.)
	P-10	Rheological analysis of Ni-rich cathode slurries with oxalic acid additive for controlling gelation	Jimin Kang (Korea Univ.)
	P-11	Thermal effect on shear-induced particle migration in colloidal suspensions under planar Poiseuille flow	Jung Hwan An (Korea Univ.)
	P-12	Rheological Analysis of Battery Electrode Slurries: Effects of Conducting Additives Composition and Mixing Conditions	Kimin Kim (Soonchunhyang Univ.)
	P-13	Effect of Ethanol on the Rheological properties of Lithium-ion Battery Anode Slurries	Min Seo Park (Pusan National Univ.)
	P-14	The influence of fluid viscosity on the deposition characteristics of colloidal particles suspended in Newtonian and non-Newtonian fluids	Minsun Hwang (Dankook Univ.)
	P-15	Evaluation of Dual Curable Initiators by Photo Rheometer	Shin-nosuke Nagasaki (Kanazawa Univ.)

Location : Lobby of Conference Hall (5th floor)

Time	No.	Title	Presenter
16:15-17:45 (90min)	P-16	Photo-induced phase separation to create porous coatings: effect of particle addition	So Sato (Kyushu Institute of Tech.)
	P-17	Production of direct joining specimens of metal and resin by the fused filament lamination (FFF) method	Soma Kojitani (Kanazawa Univ.)
	P-18	Direct imaging of liquid crystal orientation near a contact line	Taichirou Senoo (Kyushu Institute of Tech.)
	P-19	Stability of the conductive path formed in AB slurries under shear flow - rheo-impedance study -	Toshiki Tanisada (Kobe Univ.)
	P-20	Preparation of Cu-based p-type oxide semiconductor thin films for energy devices	Tsubasa Otsuki (The Univ. of Tokyo)
	P-21	Nanoindentation of porous polymer-ceramic composite coatings	Wataru WAKAYAMA (Kyushu Institute of Tech.)
	P-22	Simulation study of the crystallinity on the colloidal film in drying process	Yeji Kim (Hankyong National Univ.)
	P-23	Rheo-impedance behavior of inkjet inks during drying process	Yoshifumi Yamagata (Anton Paar Japan K.K.)
	P-24	Analysis of Mechanical Properties of PVDF-HFP Polymer Binders by Molecular Dynamics Simulation	Seung Weon Jeong (Ewha Womans Univ.)
	P-25	Decomposition mechanism of fluoro-ketone as C ₃ F ₆ O: alternative film etching gas	Minji Kim (Ewha Womans Univ.)
	P-26	A Study on the Gas Decomposition Pathway Analysis for the Development of Fluorocarbon Film Deposition and Etching Process Using alternative Low-GWP Gas	Mihyeon Jo (Ewha Womans Univ.)

Study on the dispersion states of carbon particles and ionomer in water/alcohol solvents using time-domain NMR

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Abstract

Catalyst layers of polymer electrolyte fuel cells are produced by coating and drying catalyst ink, a dispersion of catalyst particles and ionomer in a water/alcohol solvent. Nafion, a typical ionomer, is reported to form primary aggregates at a low concentration and to be highly entangled with each other as increasing the concentration. In this study, the dispersion states of carbon particles and Nafion in water/alcohol solvents were meticulously investigated by using time-domain NMR (TD-NMR). TD-NMR captures the relaxation behavior of the magnetization of protons contained in water or alcohol molecules, and the proton of solvents constrained on particles or ionomers exhibits rapid relaxation. Even if protons exhibit multiple relaxation modes, a weighted average relaxation rate will be measured as far as they are exchanged quickly enough. Therefore, the shorter the relaxation time, the more solvent constrained. The effect of Nafion on the solvent constrained on carbon particles was discussed.

The relaxation time $T_{2,av}$ of the ionomer dispersions, consisting of Nafion and water/n-propanol (NPA) solvent, are shown in Fig. 1 as functions of the ionomer concentration. For all NPA concentrations, the relaxation time showed a maximum at an ionomer concentration of approximately 1 wt%. Below the criteria, it is presumed that alcohol preferentially adsorbed on primary aggregates of ionomer, and the reduction of the alcohol fraction in the solvent increased the relaxation time. On the other hand, at higher concentrations, ionomer aggregates form highly solvated secondary aggregates, which constrained a considerable number of solvent molecules and decreased the relaxation time.

Catalyst inks were prepared by dispersing carbon particles and Nafion in a water/NPA/ethanol solvent. The discussion above suggests that carbon particles are dispersed into highly entangle Nafion in the ink. TD-NMR measured a weighted average relaxation rate of free solvent ($1/T_{2,F}$) and constrained solvent on particles ($1/T_{2,C}$) for the ink. If the particle concentration (C_C) is sufficiently low, the relationship in Eq. (1) is obtained with a parameter κ , the mass ratio solvent constrained to carbon particles [1].

$$\frac{1}{T_{2,av}} - \frac{1}{T_{2,F}} = \frac{\kappa}{T_{2,C}} C_C \quad (1)$$

The relaxation rate difference between the catalyst ink and ionomer dispersion or solvent was plotted against the particle content, as shown in Fig. 2. Regardless of the addition of ionomer, a good linear relationship was obtained, as predicted from Eq. (1), and the slope, which is proportional to the mass fraction of solvent adsorbed, was hardly affected. It is clarified that the ionomer is hardly adsorbed on the surface of the carbon particles.

Keywords: catalyst ink, carbon particles, ionomer dispersion, Nafion, relaxation time

References

- [1] G. P. van der Beek, M. A. Cohen Stuart, and T. Cosgrove, "Polymer Adsorption and Desorption Studies via ¹H NMR Relaxation of the Solvent", *Langmuir* 7 (1991): 327-334

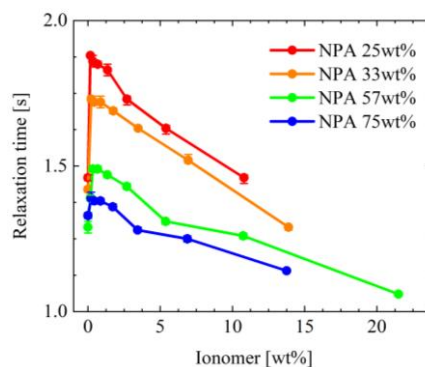


Fig. 1 Relaxation time of ionomer dispersions

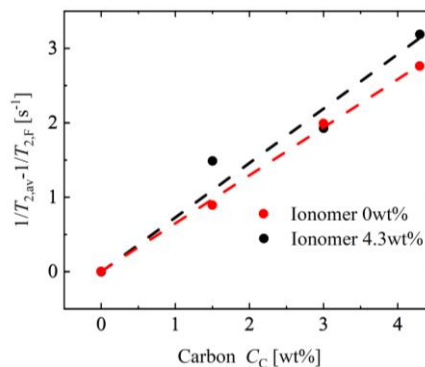


Fig. 2 Effect of carbon concentration on the mass fraction of solvent constrained

Evaluation of dual-curing initiators by real-time FT-IR

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Abstract

Dual-curing initiators (DI) are compounds with a molecular structure that decompose under ultraviolet (UV) light and heat to generate radicals and have dual functions as photoinitiators and thermal polymerization initiators. It is known that DI can be used as a polymerization initiator for acrylic and methacrylic monomers and is expected to be used in a wide range of applications requiring dark curing because it can promote polymerization curing by heating in places where UV light cannot reach or for adhesives temporarily fixed with UV light. However, the details of how much the decomposition of initiators by UV and heat contribute to the polymerization curing of monomers have not been clarified, as precise measurements have not been conducted.

This study measured and analyzed the UV- and heat-induced dual curing process using real-time Fourier transform infrared spectroscopy (RT-FT-IR, VERTEX 70, Bruker). Two different DIs, PERDUALTMTX and PERDUALTMTB from NOF CORPORATION in Japan, were used. Diurethanedimethacrylate monomer was mixed with either DI with a weight ratio of 97:3. UV light was supplied by a high-pressure mercury lamp. A photometer was used to measure the UV intensity at 365 nm. Heating was performed from 30 to 120 °C at 1.5 °C/s in the case of dual curing. Figure 1 shows the C=C bond conversion after 200 seconds since UV irradiation stopped UV irradiation and UV irradiation with heating. The results clarified that dual curing of UV irradiation and heating enhanced polymerization when the results of dual and UV curing were compared.

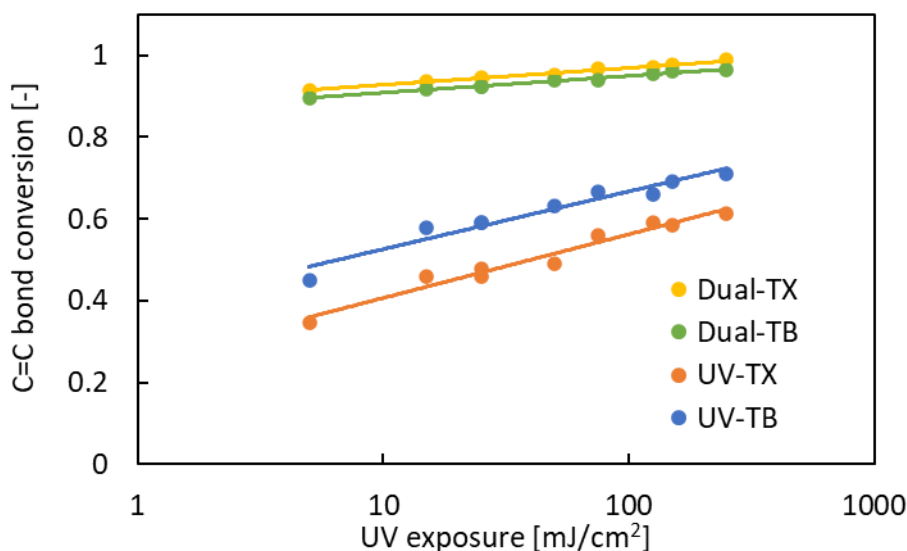


Figure 1. Effect of UV exposure on the C=C bond conversion after 200 s since UV irradiation stopped.

Keywords: Photo initiator, Thermal polymerization initiator, Dual-curing initiator, Decomposition, R-FT-IR

PERDUAL is a registered trademark of NOF CORPORATION in Japan.

References

Taki, K *Macromolecules* 47(6), 1906-1913. (2014)

Utilizing a data-driven model for numerical simulation of non-isothermal polymer melt flow

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Abstract

For both mechanical and chemical recycling waste plastics, extrusion is being posed as an efficient method to melt and transform the wastes into the recycled materials and/or into the chemical feedstocks. However, high shear forces and above-melt temperature conditions may cause mechanical degradation and uneven polymer flow. In addition, complex rheological properties of molten plastics, including shear thinning and thermal dependency of the viscosity, which make it difficult to control melt flow. In this regard, computational fluid dynamics (CFD) simulations would be helpful to analyze the flow of molten plastics [1].

Previous CFD simulations of polymer flow have used viscosity models that consider the momentum and temperature dependence simultaneously, however, we found that these existing methods may occur mispredictions at certain points. To compensate for these issues, our approach is to find the viscosity at a certain shear rate and temperature by using the multivariate interpolation, computed from several shear viscosity curves [2] at different temperatures. Using this approach, we performed numerical simulations of non-isothermal flow of low-density polyethylene (LDPE) in a 2D rectangular channel and a single-screws extruder. A commercial software based on the finite element method (FEM) was used in our numerical simulation.

Under the heating conditions, a thin thermal boundary layer forms when polymer melt flows, due to the properties of the molten plastics such as high viscosity and low thermal conductivity. This leads to a rapid decrease in viscosity and the development of uneven flow. At high flow rates and elevated heating conditions, significant differences in the flow and heat transfer characteristics such as velocity profile, pressure drop, and thickness of thermal boundary layer were observed due to the difference in the viscosity models. We observed that differences in viscosity models have a significant impact on the non-isothermal polymer melt flows and confirmed the importance of using accurate viscosity models in extrusion processes.

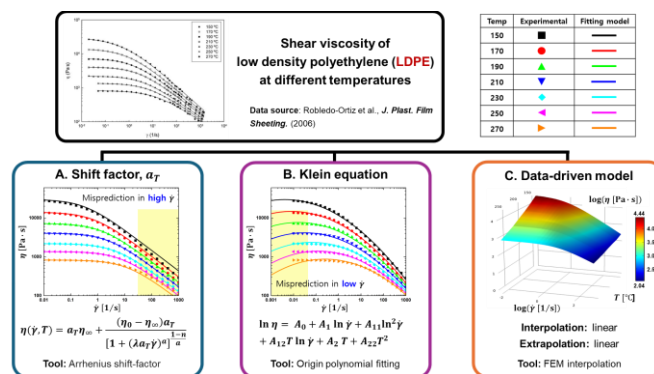


Figure 1. Viscosity models of polymer melt

Keywords: recycling waste plastics, polymer melt, viscosity model, computational fluid dynamics, single screw, non-isothermal flow

References

- [1] K. Wilczyński, A. Nastaj, A. Lewandowski, K.J. Wilczyński, K. Buziak, *Fundamentals of global modeling for polymer extrusion*. Polymers, 11(12), 2106, (2019).
- [2] J.R. Robledo-Ortiz, D.E. Ramírez-Arreola, R.G. González-Núñez, D. Rodrigue, *Effect of freeze-line position and stretching force on the morphology of LDPE-PA6 blown films*. J. Plast. Film Sheeting, 22(4), 287-314, (2006).

Investigation of hydrodynamic for viscoelastic fluid using Lattice Boltzmann Method

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Abstract

Lattice Boltzmann Method (LBM) is a technique for simulating continuum fluids by discretizing time and space using particle distribution function f , which normalize the probability that microscopic coarse-grained particles exist between lattices. Originated from physical theory of gases, such as Lattice Gas Automata (LGA), this method combines Newtonian dynamics of solid particles with a discretized Boltzmann equation for fluid phase [1].

LBM has its advantages of simplicity in their formulation and versatility. For simplicity, LBM can simulate the motion of fluid particles with only two successive procedures: particle propagation and collision. And for versatility, LBM can apply to turbulent flow, multiphase flow, but LBM specializes in simulation of colloid/suspension fluids [2]. In this paper, we will describe viscoelastic fluid with hard-sphere suspension system to investigate the influence of hydrodynamic interaction and stress caused by polymeric solvent considering fluid-particle interactions (e.g. Oldroyd-B solvent with particles) and particle-particle interactions (e.g. attractive/repulsive force). Our study provide insights which can ultimately aid in optimizing process for dealing with suspension flows.



Figure 1. Interactions between two particles at a fluid-fluid interface [3]

Keywords: Computational fluid dynamics, finite difference method, Lattice Boltzmann method, viscoelastic fluid

References

- [1] Cyrus K. Aidun and Jonathan R. Clausen, 'Lattice-Boltzmann Method for Complex Flows', Annual Review of Fluid Mechanics 42, 439-472 (2010).
- [2] Mewis, Jan, and Norman J. Wagner. 'Colloidal suspension rheology'. Cambridge university press, 2012.
- [3] Onishi, Junya, et al. "Lattice Boltzmann simulation of capillary interactions among colloidal particles." *Computers & Mathematics with Applications* 55.7 (2008): 1541-1553.
- [4] Malaspinas, Orestis, N. Fiétier, and M. Deville. "Lattice Boltzmann method for the simulation of viscoelastic fluid flows." *Journal of Non-Newtonian Fluid Mechanics* 165.23-24 (2010): 1637-1653.

Dispersion process of silica particles in epoxy resin using a planetary centrifugal mixer based on energy balance equation

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Abstract

Silica-filled epoxy resin is frequently utilized to fill the gap between the IC tip and the wafer to protect the wiring with small thermal expansion. Since particle aggregates cause the gap clogging and viscosity increase, leading to an insufficient filling, a uniform dispersion of silica particles in the resin matrix is required. A planetary-centrifugal mixer is often used to prepare such a mixture, but the details of the dispersion process have not been clarified. Our group proposed a method to estimate the shear rate in a vessel based on the temperature change and energy balance equation [1]. This study utilized the same temperature measuring devices to estimate the amount of heat generated by the friction between particles and discuss the progress of particle dispersion.

Figure 1 presents the variations in air and mixture temperatures in the redispersion process of the silica filled epoxy resins at different silica particle volume fractions (20 and 50vol%). Notably, both temperatures exhibited a monotonic increase at 20vol%, while a two-stage temperature increase was observed at 50 vol%. This finding is significant as it suggests a distinct rheological change in the mixture at the higher particle volume fraction, potentially influencing the dispersion process.

Frictional heat Q_F was calculated from the energy balance equation, shown as Eq. (1). LHS represents the accumulation term, which is the product of the heat capacity of the mixture and the gradient of fluid temperature, T . RHS consists of viscous dissipation, conductive heat, and frictional heat terms. The viscosity in the viscous dissipation term was calculated considering the silica volume fraction and the temperature during dispersion process. The mean shear rate in a vessel was estimated according to the procedure proposed in our previous study [1], considering the mixing condition.

$$\left(\rho_m C_{p,m} V(1 - \phi) + \rho_s C_{p,s} V\phi\right) \frac{dT}{dt} = V\eta\dot{\gamma}^2 + U_G A_G (T_G - T) + Q_F \quad (1)$$

Figure 2 represents the changes in the estimated frictional heat for both silica-filled epoxy resins. At 20 vol%, the frictional heat was observed only for the first 60 s. A zero frictional heat after that indicates that silica particles are entirely dispersed and isolated from each other in the resin matrix. At 50vol%, however, the frictional heat was negative for 120 s. Although the mixture initially behaves as an elastic solid and the shear rate must be very small, the viscosity of the mixture was calculated considering the temperature only. Therefore, the procedure proposed in ref [1] overestimated the mean shear rate, which causes negative frictional heat. As time passed with temperature increase, the mixture became viscous dominant and was fluidized in the vessel, generating frictional heat. As a result, the frictional heat took the maximum at 200 s, where the temperature-increasing behavior was changed. After that the frictional heat was slowly decreased to zero compared with the 20vol% mixture. Since no frictional heat is observed after 700 s, silica particles can be separated from each other.

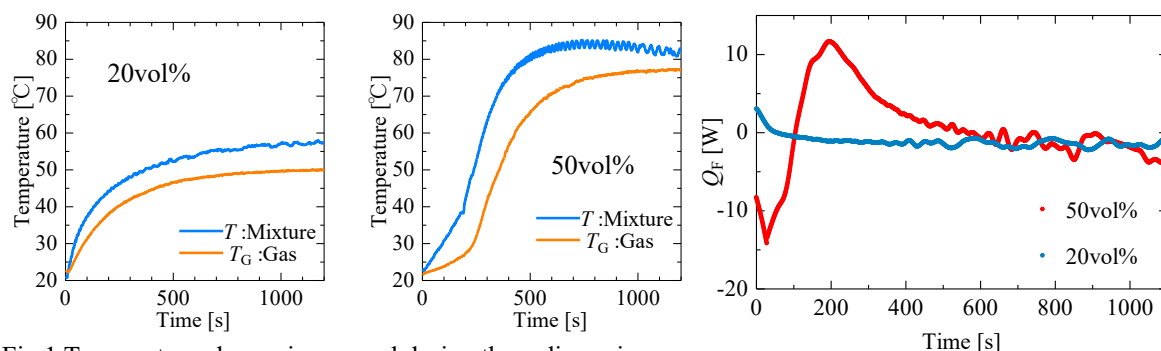


Fig.1 Temperature change in a vessel during the redispersion process of silica-epoxy mixtures

Fig.2 Frictional heat in the redispersion process of silica-epoxy mixture

Keywords : planetary centrifugal mixer, Silica-epoxy resin, shear rate, energy balance equation

References [1] Komoda, et al., *Chem. Eng. Res. Des.*, **202**, 355-364 (2024)

Influence of hydrodynamic interaction on stratification during film drying process: Effects of particle size ratio

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Abstract

Drying processes of colloidal suspensions are commonly employed in various industrial applications such as functional films, battery electrodes, and coating materials. During the drying process of colloidal suspensions, colloidal particles tend to accumulate near the interface when evaporation dominates, while they are distributed uniformly when Brownian motion dominates. Size-dependent stratification may occur during the drying of two types of particles with different sizes. The key factors governing this stratification include the evaporation rate, particle size ratio, and initial composition.

In this study, simulations using the lattice Boltzmann (LB) method were conducted to investigate the effect of hydrodynamic interactions (HI) on the tendency for stratification of binary colloidal system [1]. The different-sized colloidal particles were constructed as raspberry by arranging point beads on their spherical shell. The motion of beads was coupled to the LB fluid, effectively reproducing hydrodynamics in the Stokes regime. To precisely analyze diffusiophoresis, where the concentration gradient of small particles influences the movement of the larger particle [2], the system was designed as a single large particle was included within a film dominated by small particles. It was confirmed that as drying progressed, the concentration development of small particles pushed larger particle downward.

Under various size ratio conditions, the effect of HI on the drying pattern was quantified, compared to the results of Langevin dynamic simulations that were modeled via implicit solvent. Additionally, the results were compared to a previous model that predicted an increase in the tendency of small-on-top as the drying speed and size ratio increase [3].

Keywords: hydrodynamic interaction, film drying, stratification, lattice Boltzmann method, Brownian motion, size ratio

References

- [1] J. S. Park, J. Yun, B. Chun, and H. W. Jung, *Mild stratification in drying films of colloidal mixtures*. *Soft Matter*, 18, 3487–3497 (2022).
- [2] A. Fortini, I. Martín-Fabiani, J. L. De La Haye, P. Dugas, M. Lansalot, F. D’Agosto, E. Bourgeat-Lami, J. L. Keddie, and R. P. Sear, *Dynamic stratification in drying films of colloidal mixtures*. *Phys. Rev. Lett.*, 116, 118301 (2016).
- [3] J. Zhou, Y. Jiang, and M. Doi, *Cross interaction drives stratification in drying film of binary colloidal mixtures*. *Phys. Rev. Lett.*, 118, 108002 (2017).

How to accurately measure the maximum adhesion force of a liquid on a solid surface

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Abstract

Coating is a scientific process that is widely used. From printing and paint in our lives to the spin coating process of semiconductor technology, or surface modification technology, the existence of coating technology can be seen. Measuring the friction between liquid and solid surfaces can explain coating technology from a more basic physical mechanism and has the potential to enhance the progress of coating technology. So the theory of coating wetting was explored and calculated, and finally it was concluded by [1]~ [3], that $F = kW\gamma_{LV}(\cos\theta_R - \cos\theta_A)$.

The Droplet Adhesion Force Instantaneous Measurement System (DAFI) can accurately and quantitatively measure the interaction force between liquids and solids. Pilat et al. (2012) [4] first used a glass capillary as a cantilever beam (Droplet Adhesion Force Instantaneous Measurement System, DAFI) to pulling a droplet and measure the deformation of the beam, to measure the wettability characteristics of low contact hysteresis angle surfaces. Gao et al. (2018) [5] found that before the liquid start to move on the solid surface, it must first break through the maximum adhesion force (F_s) and then reach the dynamic equilibrium adhesion force (F_d). Lai (2023) [6] conducted systematic experiments on experimental parameters that were not discussed in many references and confirmed that to accurately measure the maximum adhesion force of a liquid on a solid surface, it is necessary to clearly explain the droplet beam contact method and beam height in DAFI system, also measured adjustment parameter k equal to 1 through the DAFI system, and used this formula to calculate the force required to wet the liquid on the solid surface.

This article further studies the impact of the surface hydrophilicity and coating status of the beam in the DAFI system on the measurement results. The results show that if the beam surface is hydrophobic, the experiment will not be able to obtain continuous measurement results (drop will peel off from the beam), also the hydrophobicity of the beam will affect the initial state of the droplet, thereby affecting its measurement results. Therefore, we can make this measurement system more stable and the measurement results more accurate.

Keywords : Interface mechanics measurement, DAFI, Maximum adhesion force

References

- [1] Rosano, H. L. (1951). Mem. Services Chim. Etat. : 437
- [2] Furmidge, C. G. L. (1962). "Studies at phase interfaces. I. The sliding of liquid drops on solid surfaces and a theory for spray retention." Journal of Colloid Science 17(4): 309-324.
- [3] Extrand, C. W. and Y. Kumagai (1995). "Liquid Drops on an Inclined Plane: The Relation between Contact Angles, Drop Shape, and Retentive Force." Journal of Colloid and Interface Science 170(2): 515-521.
- [4] D. W. Pilat, P. Papadopoulos, D. Schäffel, D. Vollmer, R. Berger, and H.-J. Butt (2012). "Dynamic Measurement of the Force Required to Move a Liquid Drop on a Solid Surface." Langmuir
- [5] Nan Gao, Florian Geyer, Dominik W. Pilat, Sanghyuk Wooh, Doris Vollmer, Hans-Jürgen Butt & Rüdiger Berger (2018). "How drops start sliding over solid surfaces." Nature Physics
- [6] Liang-Je Lai (2023). "Analysis of Drop Adhesion Force Instrument (DAFI) and its application for the onset of drop on a solid surface" Master Thesis

Assessing the impact of slurry mixing conditions on Electrochemical Lithium Recovery (ELR) system performance

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Abstract

In today's rapidly growing battery market, which includes small batteries, electric vehicles (EVs), and energy storage systems (ESS), securing a steady supply of lithium, the primary raw material for batteries, has become important. However, current lithium production technologies are expected to be inadequate to meet the anticipated demand for lithium. Given these circumstances, the Electrical Lithium Recovery (ELR) system has attracted attention. ELR system utilizes LMO (Lithium Manganese Oxide) electrodes to selectively extract lithium from seawater or wastewater through the charging and discharging principles of the electrodes. This technology is more environmentally friendly compared to conventional methods and offers the advantage of flexible production speed control. While previous research has primarily focused on electrode materials and operational conditions for ELR systems [1], the electrode manufacturing process should be crucial to determine the system performance, as shown in other electrode systems [2].

This study aims to investigate the influence of mixing conditions, among other electrode manufacturing variables, on the performance of ELR systems. Cathode slurry incorporating LMO as the active material was prepared at various mixing conditions of a planetary mixer used for slurry preparation. We confirmed that rheological properties of the cathode slurries vary depending on the mixing conditions. Subsequently, we coated the manufactured slurry onto carbon sheets and assembled it into a wet cell configuration using LiCl as the electrolyte to measure the electrode performance accordingly. We aimed to identify the correlation between the changes in rheological properties and electrode performance. This study is expected to serve as an initial step to design advanced ELR systems, focusing on the importance of the process technologies on the final system performance.

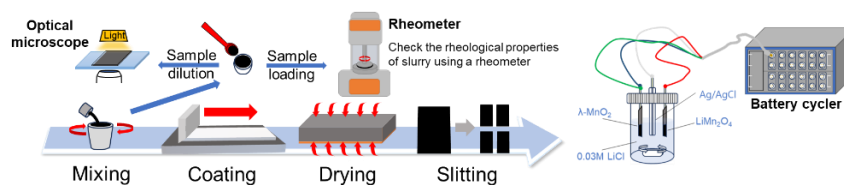


Figure 1. Electrode manufacturing and characterization procedure

Keywords: Lithium, Electrochemical lithium recovery (ELR) system, Slurry mixing, Lithium manganese oxide, Electrode manufacturing

References

- [1] H. Joo, J. Lee, J. Yoon, *Short review: timeline of the electrochemical lithium recovery system using the spinel LiMn_2O_4 as a positive electrode*. *Energies*, 13(23), 6235 (2020).
- [2] T. Mori, T. Ochi, K. Kitamura, *Characterization of slurries for lithium-ion battery cathodes by measuring their flow and change in hydrostatic pressure over time and clarification of the relationship between slurry and cathode properties*, *J. Colloid Interface. Sci.*, 629, 36-45 (2023).

Investigation of Flow Field Variation in Multilayer Slot Coating

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Abstract

Coating technology is crucial in industry today, widely used for treating surfaces and making specialized coatings. In the realm of coating technology, slot coating stands out due to its extensive utilization for surfacing materials with specific performance requirements. Its advantage lies in its ability to control film thickness through experimental conditions such as flow rate and coating speed. However, there remains a relatively limited understanding of the fluid dynamics variation during multilayer slot coating processes. Therefore, this study aims to investigate the impact of different coating material properties on flow field distribution in multilayer coating scenarios. This research adopts numerical simulation methods to systematically study flow field variations during the processes of multilayer slot coating. A computational model will be established, encompassing the surface tension, slot effects, and Volume of Fluid (VOF), to investigate the changing patterns of flow fields during slot coating. The outcomes of this research will contribute to the better understanding of fluid dynamics in multilayer coating processes, thereby improving product quality and performance.

Keywords : Slot coating, multilayer coating, numerical simulation

Rheological analysis of Ni-rich cathode slurries with oxalic acid additive for controlling gelation

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Abstract

High-Ni layered oxide cathodes are required in battery industry for their high energy density. However, increasing the content of nickel leads to defects of cathode slurry. When the cathode slurry is exposed to moisture and CO₂ in the ambient air, residual lithium (LiOH, Li₂CO₃) is formed on the surface of the cathode material, causing an alkaline environment in the cathode slurry [1]. Polyvinylidene fluoride (PVDF), which is a polymer binder, undergoes dehydrofluorination reaction due to its vulnerability in alkaline conditions. This reaction triggers the formation of conjugated C=C bond and crosslinks between PVDF chains, leading to gelation [2]. To ensure the uniform coating layer of electrodes in the manufacturing process and the high performance of battery, it is crucial to prevent the gelation of the slurry.

In this study, oxalic acid was employed as an organic acid additive for preventing gelation in the Ni-rich cathode slurry by neutralizing alkaline environment. The role of oxalic acid in cathode slurry system in hindering gelation mechanism was examined via rheological measurements. The rheological properties of slurries were measured by altering the oxalic acid content, directly reflecting the hydrogen bonding between carboxylic acid group of oxalic acid and the fluorine of PVDF [3]. The gelation behavior was monitored for 3 days by comparing the rheological properties of the reference slurry and slurry with oxalic acid. The rheological and zeta-potential data related to gelation phenomena confirmed that the gelation was notably delayed with increasing the portion of oxalic acid. Oxalic acid can play a key role in improving coating processability and performance by overcoming gelation issue in Ni-rich cathode slurry.

Keywords : Ni-rich cathode slurry, residual lithium, gelation, oxalic acid, rheological properties

References

- [1] W. M. Seong, Y. Kim, and A. Manthiram, *Impact of residual lithium on the adoption of high-nickel layered oxide cathodes for lithium-ion batteries*, Chem. Mater., 32(22), 9479-9489 (2020).
- [2] J. E. Marshall, A. Zhenova, S. Roberts, T. Petchey, P. Zhu, C. E. Dancer and V. Goodship, *On the solubility and stability of polyvinylidene fluoride*, Polymers, 13(9), 1354 (2021).
- [3] C. Ye, Q. Yu, T. He, J. Shen, Y. Li, and J. Li, *Physical and rheological properties of maleic anhydride-incorporated PVDF: Does MAH act as a physical crosslinking point for PVDF molecular chains?*, ACS Omega, 4(25), 21540-21547 (2019).

Thermal effect on shear-induced particle migration in colloidal suspensions under planar Poiseuille flow

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Abstract

Shear-induced particle migration phenomenon poses a significant challenge in coating industries that handle polydisperse suspensions, such as those involved in manufacturing electrodes for lithium-ion secondary batteries. Consequently, numerous studies have aimed to elucidate the characteristics of particle migration. One notable investigation by Chun et al. [1] utilized lattice Boltzmann simulation to explore the behavior of non-colloidal monodisperse suspension systems under Poiseuille and Couette flows. They demonstrated that particles migrate towards the mid-plane of the channel in Stokes regime under Poiseuille flow condition. Additionally, Chun et al. [2] investigated non-colloidal bidisperse suspensions under Poiseuille flow, exhibiting size segregation as well as particle migration. The difference in entrance length between larger and smaller particles causes larger particles to migrate towards the center region while smaller particles are excluded from it, moving toward walls.

Colloidal particles small enough to be affected by the thermal effect exhibit Brownian motion. This thermal-induced motion results in particles moving from regions of high concentration to low concentration, which leads to the opposite of shear-induced migration. This study deals with simulation of colloidal suspensions under planar Poiseuille flow, employing the lattice Boltzmann method. To incorporate thermal fluctuations into the simulation, we introduced random fluctuations to the stress tensor at each fluid node. When considering a particular thermal fluctuation factor, results revealed that Brownian motion disrupts shear-induced migration, relaxing an inhomogeneous concentration profile. This observation aligns with experimental results from Semwogerere and Weeks [3]. Furthermore, by varying the Peclet number, which means a ratio of convection and diffusion, we can investigate the thermal effects on shear-induced migration in colloidal suspensions.

Keywords: particle migration, colloidal suspension, Poiseuille flow, lattice Boltzmann method, Brownian motion, thermal effect, Peclet number

References

- [1] B. Chun, I. Kwon, H.W. Jung, and J.C. Hyun, *Lattice Boltzmann simulation of shear-induced particle migration in plane Couette-Poiseuille flow: Local ordering of suspension*, Phys. Fluids, 29(12), 121605 (2017).
- [2] B. Chun, J.S. Park, H.W. Jung, and Y. Won, *Shear-induced particle migration and segregation in non-Brownian bidisperse suspensions under planar Poiseuille flow*, J. Rheol. 63(3), 437 (2019).
- [3] D. Semwogerere, and E.R. Weeks, *Shear-induced particle migration in binary colloidal suspensions*, Phys. Fluids, 20(4), 043306 (2008).

Rheological Analysis of Battery Electrode Slurries: Effects of Conducting Additives Composition and Mixing Conditions

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Abstract

The rheological characteristics of the battery electrode slurries have a significant impact on determining the microstructure and efficiency of battery cell manufacturing. Anode slurries with rheological properties are crucial to understanding the fundamentals behind the high performances of the electrodes, which could include dispersion, microstructure, and so on during the manufacturing process. To address these issues, we need to study the fundamental characteristics of slurry by conducting rheological experiments with changes in various parameters (composition, material, etc.) and investigating the interactions between them.

In this study, we conducted the following three tests: Amplitude sweep, Frequency sweep, and Shear sweep for CB (Carbon Black) slurry with various composition sets. The results were analyzed using the Ellis model combined with yield stress by regression fitting. Additionally, to examine the dispersion issues with respect to the conducting additives, we performed a frequency sweep test of the slurries according to the mixing time not only for CB but also for CNT (Carbon nanotube).

As a result, we were able to understand the interaction between solvents and components by deriving rheological data on the slurry. Furthermore, we found an appropriate mixing time for uniform dispersibility depending on the materials. This research will lead to promoting rheological understanding and contribute to reducing various issues in the battery production process.

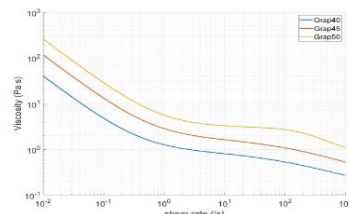


Figure 1. Rheology data graph according to graphite composition

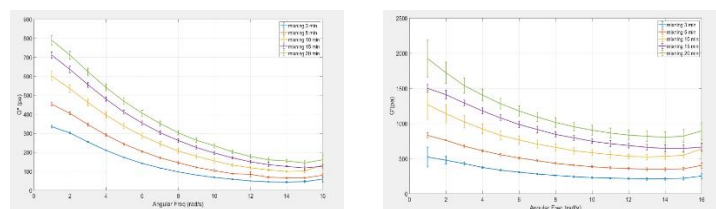


Figure 2. G', G'' graph of CNT suspension according to mixing time

Keywords: Rheological analysis, Battery electrode slurries, Conductive additives, Mixing condition

References

- [1] Carl D. Reynolds, Sam D. Hare, Peter R. Slater, Mark J. H. Simmons, and Emma Kendrick, *Rheology and Structure of Lithium-Ion Battery. Energy Technology*, **10**, 2200545, 1-13 (2022).
- [2] Jeong Hoon Park, Sang Hoon Sung, Sun Hyung Kim, Kyung Hyun Ahn, *Significant Agglomeration of Conductive Materials and the Dispersion State Change of the Ni-Rich NMC-Based Cathode Slurry during Storage*, *Ind. Eng. Chem. Res.*, **61**, 2100–2109, (2022)

Effect of Ethanol on the Rheological properties of Lithium-ion Battery Anode Slurries

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Abstract

The production process of lithium-ion batteries encompasses various stages, including mixing, coating, drying, and so on [1]. Among these, the drying process is known to be energy-intensive and costly. This is because it requires fast turnaround times, and it is carried out at high temperatures to quickly evaporate the solvent. It is well-known that water is commonly used as a solvent in anode slurry manufacturing. In this study, it was noted that the speed of the drying process can be improved by adding ethanol to water. Improved drying speed will reduce energy consumption for solvent removal and enhance economic efficiency in anode production.

The drying process is a multifaceted process involving not only heat transfer but also mass transfer from materials that make up the slurries, such as particles, binders, and solvents. Within this process, solvent evaporation, binder diffusion, and particle sedimentation occur [2]. Additionally, ethanol will affect microstructure of anode slurry. Therefore, in this study, we not only measured the drying rate of the slurries containing ethanol as a solvent but also investigated the rheological properties to have insight into the microstructure of the slurries.

To prepare the anode slurries, we used two types of graphite (spherical and flake shape) as active materials, carbon black as a conductive agent, and carboxymethyl cellulose (CMC) as a polymer binder. And we adjusted the water-to-ethanol ratio used as a solvent to 5:5, 6:4, 7:3, 8:2, 9:1, and 10:0. First, we investigated the microstructure of slurries using an optical microscope (OM) to observe the dispersion of particles. Secondly, the drying rate of the slurries was measured at room temperature. Finally, the steady shear test and small amplitude oscillation shear (SAOS) test were performed to investigate the thixotropy, rheological hysteresis properties, and linear viscoelasticity of the slurries.

This study allowed us to understand how the addition of ethanol as a solvent affects the microstructure, drying rate, and rheological properties of slurries with different active material types. Investigating the effect of ethanol on the anode slurry is important for enhancing processability and economic efficiency in anode manufacturing.

Keywords: Anode Slurry, Electrode Rheology, Ethanol solvent

References

- [1] W. Blake Hawleya,b, Jianlin Li, *Electrode manufacturing for lithium-ion batteries—Analysis of current and next generation processing*. Journal of Energy Storage. 25, 100862 (2019).
- [2] Malcolm Stein IV, Aashutosh Mistry, and Partha P. Mukherjee, *Mechanistic Understanding of the Role of Evaporation in Electrode Processing*, Journal of The Electrochemical Society, 164(7), 1616-1627 (2017).

The influence of fluid viscosity on the deposition characteristics of colloidal particles suspended in Newtonian and non-Newtonian fluids

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Abstract

As particle suspension flows through a channel, a fraction of particles would be deposited on the channel surface, inducing particulate clogging. If this happens consistently, it may deteriorate the productivity and profitability of the corresponding processes. This has led to many studies aiming to understand the deposition phenomena under various conditions [1] and with several channel geometries [2]. Among the channel geometries, an expansion-contraction channel has utility for micro-mixing, slot die coating, and hydraulic fracturing [3], however, there has been limited studies on particle deposition in this geometry.

This study is conducted to understand particle deposition characteristics with the change of fluid viscosity in both Newtonian and non-Newtonian fluids. Glycerin aqueous solution was used as the Newtonian fluid, while the non-Newtonian fluid was prepared by adding water-soluble polymer to the glycerin aqueous solution. Polystyrene colloidal particles were suspended in both fluids and these feed solutions were injected into the expansion-contraction microchannel using a syringe pump. Observations were made using an inverted microscope and CCD camera, producing a series of 2-D images showing the progress of channel clogging. For qualitative and quantitative analysis, image processing with a Python-based code was implemented.

The increase in fluid viscosity led to a lower quantity of deposited particles in both fluids. However, the shape of the particle deposition was differed between the Newtonian and non-Newtonian fluids. Higher viscosity resulted in a greater particle deposition near the channel wall compared to the center, whereas occasional particle deposition was observed within the center in the case of the non-Newtonian sample. It was also noted that particle deposition occurred more widely inside the cavity in the non-Newtonian sample due to the flow instability of the medium. This study provides helpful insight to understand the effect of fluid viscosity on particle deposition in both Newtonian and non-Newtonian fluids.

Keywords: particle deposition, clogging, expansion-contraction channel, microfluidics, colloidal suspension, polymer solution

References

- [1] B. Dersoir, M.R. de Saint Vincent, M. Abkarian, H. Tabuteau, *Clogging of a single pore by colloidal particles*. *Microfluid Nanofluid*, 19, 953–961 (2015).
- [2] D. Y. Kim, S. Y. Jung, Y. J. Lee, K. H. Ahn, *Effect of colloidal interactions and hydrodynamic stress on particle deposition in a single micropore*. *Langmuir*, 38(19), 6013-6022 (2022).
- [3] M. K. Raihan, P. P. Jagdale, S. Wu, X. Shao, J. B. Bostwick, X. Pan, X. Xuan, *Flow of Non-Newtonian Fluids in a Single-Cavity Microchannel*. *Micromachines*, 12(7), 836 (2021).

Evaluation of Dual Curable Initiators by Photo Rheometer

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Abstract

Dual-curing initiators (DI) are compounds with a molecular structure that decompose under ultraviolet (UV) light and heat to generate radicals and have dual functions as photoinitiators and thermal polymerization initiators. It is known that DI can be used as a polymerization initiator for acrylic and methacrylate monomers. Since it can promote polymerization curing of adhesives temporarily fixed by UV irradiation and heating, it is expected to be used in a wide range of applications where dark curing is required. On the other hand, changes in physical properties due to dual curing have not been sufficiently measured or analyzed.

This study measured normal force during curing and after UV irradiation using a photo rheometer (MCR 302-WESP, Anton-Paar). PERDUAL™TX initiator was obtained from NOF CORPORATION in Japan. Diurethanedimethacrylate was mixed with the photoinitiator, PERDUAL™TX, at 97:3. The high-pressure mercury lamp was a UV light source. Fig. 1 shows the effect of UV intensity and irradiation time on the change in normal force by UV irradiation at 30°C. An increase in UV intensity and the irradiation time increases the normal force, indicating a large residual force is generated.

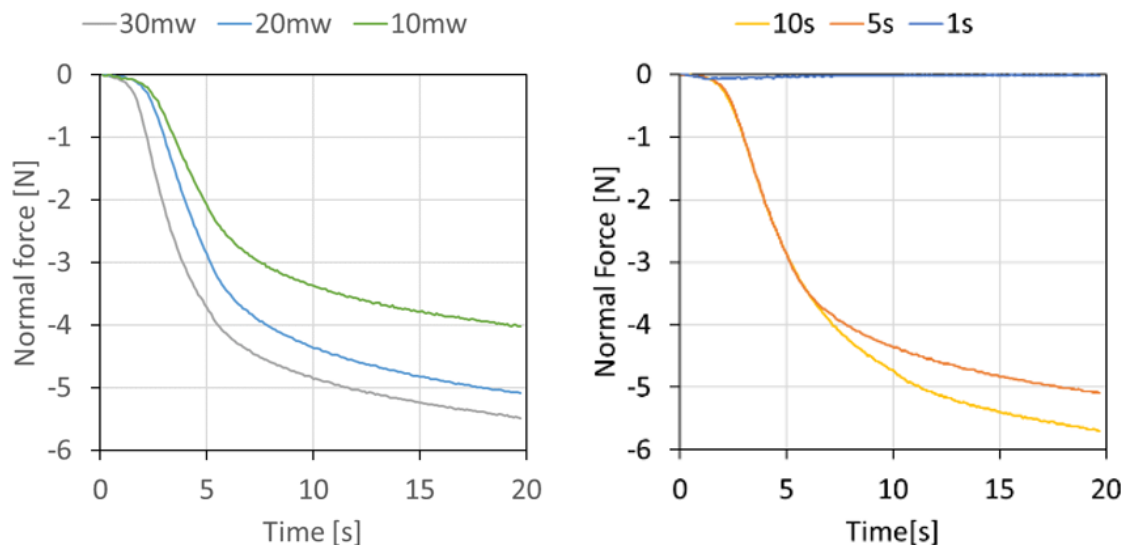


Fig. 1 Effects of (a) UV intensity at irradiation time of 5 s and (b) irradiation time at UV intensity of 20 mW/cm² on normal force.

Keywords: Dual-curing initiators (DI), ultraviolet (UV), initiators, Normal Force, Photo Rheometer

PERDUAL is a registered trademark of NOF CORPORATION in Japan.

Photo-induced phase separation to create porous coatings: effect of particle addition

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Abstract

Photopolymerization of acrylic monomers is widely used in industrial applications such as protective films and adhesives. Upon exposure to UV light, photoinitiator molecules absorb the light to generate radicals. The radicals react with the monomers and promote chain reactions to create polymers. Recently, addition of solid particles has attracted attention to achieve a high-resolution additive manufacturing^[1] and coating with a high thermal conductivity^[2].

In this study, we conducted ultraviolet curing and drying experiments of an acrylic monomer solution to create particle-loaded porous acrylic coatings using photo-induced phase separation technique. Despite previous investigations on phase separation using a polymer-incompatible solvent, it has not yet well understood how the particle loading alters the porous structures in dried coating. We aimed to clarifying the effect of the amount of silica added on the light-induced phase separation.

We used methyl ethyl ketone (MEK, Wako Pure Chemical Corporation) as solvent, polyester acrylate (M9050, Toa Gosei, Mw=1000~1500) as monomer, bis(2,4,6-trimethylbenzoyl)-phenyl phosphine oxide (Irg819, BASF) as initiator, silica particle (KE-P10, Nippon Shokubai, average diameter of 100 nm) as solid filler, respectively. The dispersions with different mass ratios of monomer:solvent:initiator:silica = 9:9:1:X (X=0-3) were prepared and applied to a glass substrate with an initial film thickness of 800 μm . The coating was pre-dried on a hot plate with a constant surface temperature of 30 °C until the solvent concentration decreased to reach 0.5 g-MEK/g-solute. The coating was exposed to LED UV light (HSL-50UV365-4UTK, CCS) from the bottom at a wavelength of 365 ± 5 nm and an intensity of 30 mW/cm². The unreacted components were then washed off by ethanol. The dried coating was peeled off from the substrate to observe the cross section using scanning electron microscope (SEM, JCM-7000, JEOL). Local thicknesses in the vertical direction relative to the bottom surface were measured at several different positions in the obtained cross-sectional image and averaged to obtain mean film thicknesses.

Fig. 1 shows the variations in dry film thicknesses with UV irradiation times for two different initial silica mass ratios. For the particle-free system (X=0), the film thickness increased linearly with the logarithm of the irradiation time. This is qualitatively consistent with the theory of Cabral et al.^[3]. In contrast, the film thickness of the particle-dispersed system (X=1) increased rapidly at a certain range of irradiation times between 1.35 and 1.4 s, indicating different growth mechanism compared to the particle-free system.

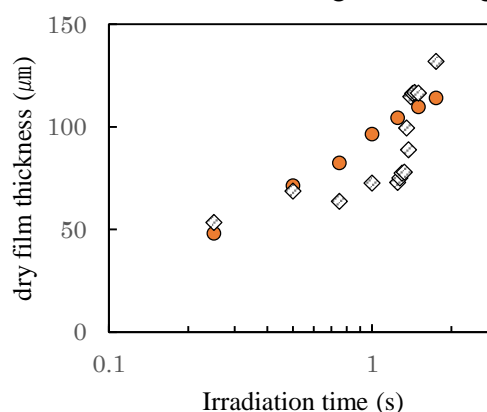


Figure 1. Relationship between irradiation time (log) and film thickness at different particle mass ratios X = 0 (circle ●) and X = 1 (◆)

Keywords: Photo-induced phase separation, particle addition, film thicknesses, UV irradiation

References

- [1] D.T. Rau et al., *Additive Manufacturing* 42 (2021) 101996
- [2] T.Y.K. Ho et al., *Additive Manufacturing* 73 (2023) 103664
- [3] J.T. Cabral et al. *Langmuir* 20 (2004) 10020-10029

Production of direct joining specimens of metal and resin by the fused filament lamination (FFF) method

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Abstract

In recent years, the development of multi-material technology has led to continued progress in molding technology for composites of a wide variety of materials. It has many advantages such as higher strength, lighter weight, optimization of functions, reduction of manufacturing costs, and diversification of designs, and has enabled the fabrication of products that meet a variety of needs. In the automotive and aircraft industries, in particular, there is a need to improve fuel efficiency and reduce weight as a countermeasure against global warming, and the use of multi-materials is a major key. To fully demonstrate the advantages of multi-materials, it is essential to establish a joining technology for reliable joining of different materials.

In the field of 3D printing, the technology for joining different materials with high-joining strength has not yet been established. In many cases, the process of creating a three-dimensional object begins with the creation of a mold, but modeling with a 3D printer does not require a mold and has advantages such as the ability to quickly realize ideas and reduce development time and costs.

This study first fabricated an Al-PA6/CF bonding specimen using the Gutenberg G-ZERO 3D printer, in which a portion of a DLAMP-treated aluminum piece was directly bonded to a carbon fiber reinforced resin (PA6/CF). DLAMP treatment is a process in which a roughened area is formed on the metal surface by laser irradiation. Next, the strength of the specimens was evaluated using a tensile tester. In addition, the bonded surfaces of the specimens were observed by X-ray CT to confirm the condition of the specimens. Specimens with a tensile strength of 20 MPa could be produced.

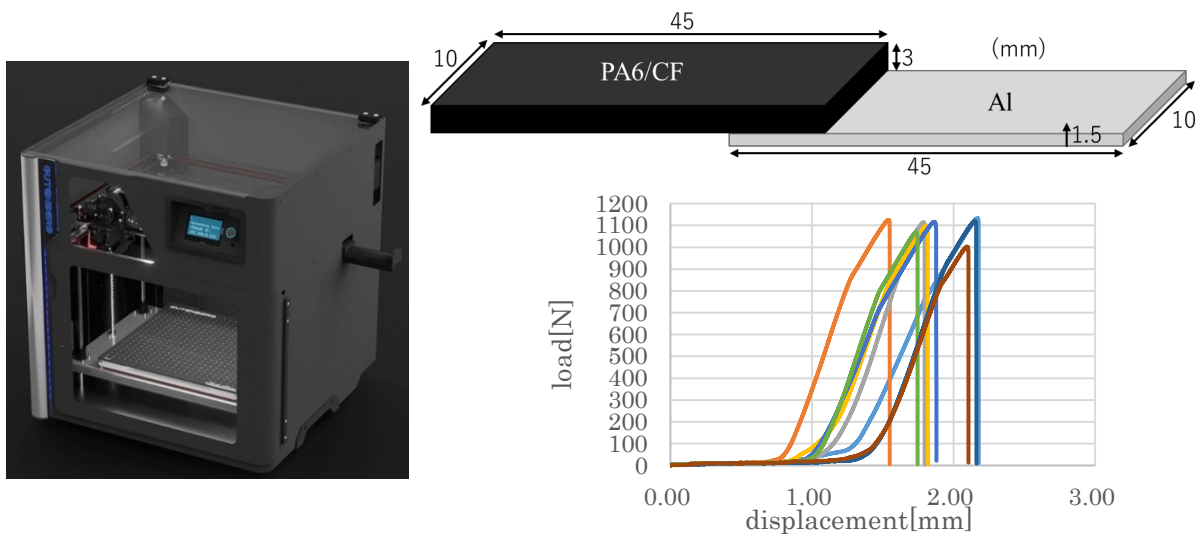


Figure 1. 3D printer, Al-PA6/CF bonding specimen, Load displacement curve

Keywords: 3D print, multi-material, DLAMP, Al-PA6/CF, joint

Direct imaging of liquid crystal orientation near a contact line

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Abstract

Isostearyl glyceryl ether (IS) forms rod-shaped inverse micelles, which self-assemble to form inverse hexagonal (H_2) lyotropic liquid crystals in the presence of water. The liquid crystals have attracted attentions in potential applications of moisturizers for pharmaceuticals and cosmetics. It is important to understand the dynamic structure changes in a drying liquid crystal near a contact line. Davidson et al.^[1] have previously reported the dynamic change in molecular orientations in an evaporation liquid crystal droplet, but their study was limited to a qualitative evaluation using polarized light microscopy. In this study, we aimed at quantitatively evaluating local liquid crystal orientation near the contact line of drying IS-water mixtures by using a two-dimensional birefringence distribution imaging system.

The measurement cell was made by sandwiching a U-shaped PC film (ASONE) between two glass plates and gluing them together with a clearance of 880 μm . We filled the cell with the IS solution to promote uni-directional water evaporation. An LED light (Photron, IBF-LX60AG, wavelength 532 ± 2 nm) was transmitted through a circular polarizing film consisting of a linear polarizer and a quarter-wave plate, and irradiated to the sample. We used a polarization image sensor (Photonic Lattice, PI-micro) composed of a pixelated polarizer array made from photonic crystals with different transmission axes of 0° , 45° , 90° and 135° [2]. The photodetector was connected to an optical lens (KEYENCE, VH-Z259) to visualize local phase differences and axial orientations with a magnification of $\times 175$.

Figure 1 shows (a) axial color maps and (b) schematic liquid crystal orientation near the contact line for the IS-water solution with an initial IS mass fraction of 82 wt% and dried at 50°C . A white region near the contact line indicates an isotropic phase with negligible birefringence at 80 minutes drying. The results revealed that layered phases with different axial orientations of approximately 135° and 45° were stacked together at the boundary between the isotropic and liquid crystalline phases, indicating unique evaporation-induced orientations of inverse micelles near the contact line.

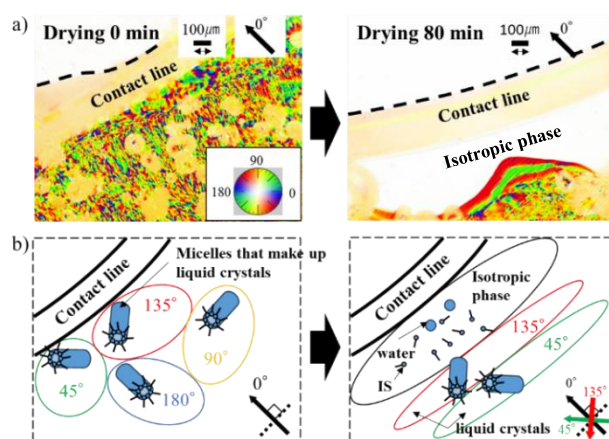


Figure 1. Changes in liquid crystal orientation during drying

a) axial color maps, b) schematic liquid crystal orientation near the contact line

Keywords : liquid crystal orientation, drying, 2D birefringence imaging, optical retardation, axial orientation

References

- [1] Z.S. Davidson et al, *Deposition and drying dynamics of liquid crystal droplets*. Nature Communications 8, 15642 (2017).
- [2] T. Onuma, Y. Otani, *A development of two-dimensional birefringence distribution measurement system with a sampling rate of 1.3 MHz*. Optics Communications 315, 69-73 (2014).

Stability of the conductive path formed in AB slurries under shear flow - rheo-impedance study -

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Abstract

Lithium-ion batteries are widely used, but further performance improvement is still needed. Excellent electrical conductivity of electrode films is essential for high-performance batteries, but the shear deformation, being subjected in the manufacturing process, affects the conductivity of the electrode and the conductive additive slurries. This study investigated the stability of the conductive paths formed in acetylene black (AB) slurry under shear flow through time-dependent AC impedance measurements.

The study used a slurry composed of AB, PVdF, and NMP, with AB concentrations of 1.2, 2.4, and 4.6wt% and a constant PVdF concentration of 8wt%. Impedance measurements were conducted by applying alternating current voltage to the AB slurry, filling the gap between inner static and outer rotational concentric cylinders. The previous study [1] revealed that the impedance at low (<100 Hz) and high (>10 kHz) frequencies can evaluate the conductive paths between cylinders and in the microstructure. The impedance was measured every 0.1 s with a stepwise change in the rotational speed of the outer cylinder, proportional to the applied shear rate.

Figure 1 illustrates the impedance variation with stepwise increase and decrease in shear rate for a 1.2wt% AB slurry. The impedance increased rapidly during the shear application but returned to the initial value after stopping the shear application. It is revealed that the micro-scale conductive paths were partially broken up under shear but reconstructed quickly. Furthermore, the impedance exhibits fluctuation with a constant amplitude during shear application. The impedance variation at the highest shear rate resembles that of the PVdF solution. These fluctuations were quantified as a coefficient of variation (CV), and the influences of AB concentration and shear rate applied are summarized in Figure 2. The impedance was low and constant at the highest AB content regardless of shear rate, with a CV of only 2%. Therefore, the micro-scale conductive path was firmly formed at this composition and was rarely destroyed under intense shear flow. However, the impedance and CV were simultaneously increased with the increase in shear rate or the decrease in AB content. It was found that conductivity became unstable when the conductive path was partially destroyed. At the highest shear rate and lowest AB content, the conductivity was comparable to that of the PVdF solution, implying that the micro-scale conductive paths were entirely destroyed.

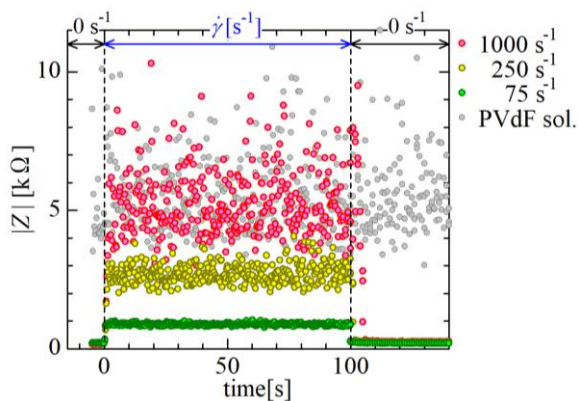


Fig.1 Variation of the magnitude of impedance with stepwise shear application (1.2wt% AB slurry)

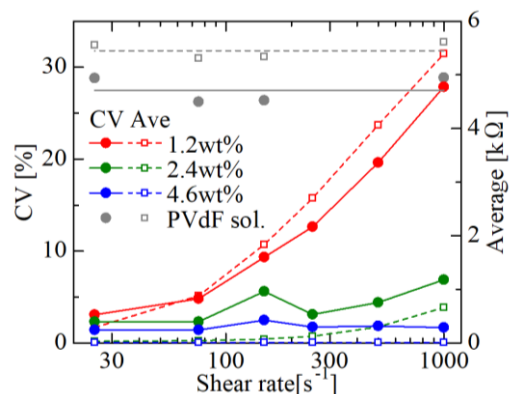


Fig.2 Effect of shear rate on the coefficients of variation and average of the magnitude of impedance.

Keywords: rheo-impedance, Lithium-ion batteries, cathode slurry

References: [1] K. Yoshida, Y. Komoda, N. Ohmura, 12th Asian Coating Workshop, Kanazawa, (2022)

Preparation of Cu-based p-type oxide semiconductor thin films for energy devices

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Abstract

Metal oxide semiconductors have been intensively studied for application in energy devices using p-n junctions, such as thermoelectric devices. However, the development of p-type semiconductor has been delayed due to its electronic configuration. The valence band maximum (VBM) of p-type oxide semiconductors consists of the strongly localized oxygen 2p band, resulting in very low carrier mobility. In 1997, Kawazoe *et al.* proposed a strategy of forming a hybridized energy level between the d level of the metal cation and the 2p level of the oxygen anion.^[1] This leads to delocalization of the VBM and, as a result, higher carrier mobility of the p-type semiconductors. In addition, the closed-shell electron configuration avoids strong coloration due to d-d transitions, resulting in high optical transparency.

We have reported Cu₂O thin film grown at 400 °C showed p-type conductivity with a carrier concentration of $4.10 \times 10^{16} \text{ cm}^{-3}$ and a hall mobility $2.07 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ^[2]. However, the electric properties of Cu₂O were unstable in the atmosphere. Cu-based delafossite oxides (CuMO₂; M = Al, Cr) are metastable phases and exhibit p-type conductivity. CuMO₂ thin films have been fabricated by various methods such as pulsed laser deposition, magnetron sputtering, chemical vapor deposition and spin coating.

In this work, we focus on ultrasonic spray deposition method. Aluminum acetylacetonate, chromium acetylacetonate and copper nitrate trihydrate were used as soluble precursors in *N,N*-dimethylformamide. Delafossite CuAlO₂ and CuCrO₂ thin films were deposited on thermally oxidized Si substrate at 400 °C and annealed at 800 °C for 2 h under nitrogen atmosphere in furnace tubing. Fig.1 shows the X-ray diffraction patterns of copper-aluminum oxide thin film as deposited and after annealed. The amorphous phase was observed in the as deposited thin film and thin film after annealing present a mixture of CuAlO₂, CuAl₂O₄ and Cu₂O phases. We will discuss the effects of deposition temperature, annealing temperature and composition ratios on Cu-based delafossite oxide thin films.

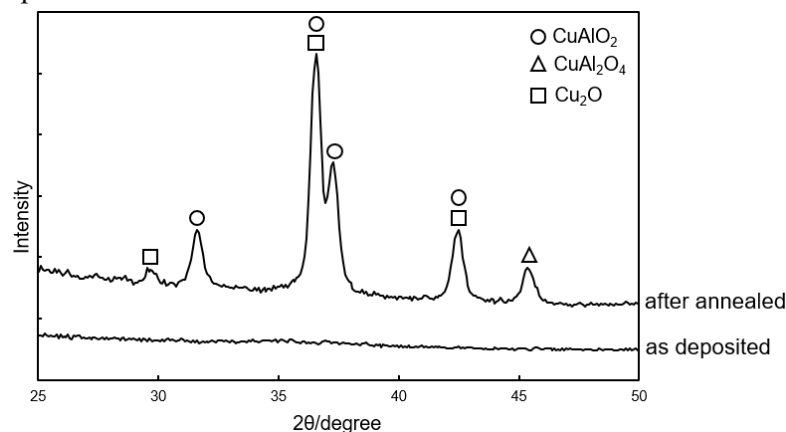


Figure 1. XRD patterns of copper aluminum oxide thin film as deposited and after annealed

Keywords: energy device, p-type semiconductor, thin film, ultrasonic spray deposition, delafossite structure

References

- [1] Kawazoe H., Yasukawa M., Hyodo H. *et al.*, *Nature* 389, 939 (1997).
- [2] "Formation of Cu₂O p-type oxide semiconductor thin films by wet process." Y. Tsuji, K. Kawamoto, 8th Asian Coating Workshop (2016).

Nanoindentation of porous polymer-ceramic composite coatings

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Abstract

Particulate coating products such as battery electrodes are produced by coating and drying a particle dispersion containing polymeric components. The particle layers are compressed by capillary pressure^[1, 2] when adjacent particles come into contact with each other during the drying process. The deformation leads to drying defects such as curling, delamination, and cracking. It is important to accurately measure the mechanical properties of particle-dispersed coatings. In this study, we aimed at measuring local Young's moduli of dried films at different initial polymer concentrations using the nanoindentation method^[3] in order to clarify how the polymer adsorption on particle surfaces affects the mechanical properties of dried coatings.

We used spherical silica particles of 2.5 μm (Nippon Shokubai, KE-P250) and 1.5 μm (Nippon Shokubai, KE-P150) in average diameters, hydroxyethyl cellulose (viscosity average molecular weights of 1,300,000 and 720,000 SigmaAldrich, HEC), and distilled water. The volume fraction of silica particles was fixed at 25 vol% and the initial HEC concentrations were varied between 0 and 0.25 wt%. Sample films were prepared by coating the prepared dispersion on a glass substrate and drying it on a heating plate with a constant surface temperature of 50 °C. A diamond Berkovich indenter with a triangular pyramid tip was mounted on an ultra-micro indentation hardness tester (Elionix, ENT-1100) and pressed into the dried sample surface. After loading the maximum load of 2.5 mN, the load was decreased to obtain a stress-strain curve. The maximum penetration depth was within 5% of the film thickness.

Figure 1 shows the variations in elastic modulus of silica particle films with polymer concentrations at different particle diameters of 2.5 μm (square) and 1.5 μm (diamond). The measured elastic moduli increased as decreasing the particle diameter at any polymer concentrations, showing a consistency with previous theory^[3]. The moduli first increased and then decreased with increasing the initial polymer concentration in the dispersions of 1.5 μm in particle diameter, indicating an optimum polymer loading to maximize the mechanical properties of dried coatings.

Keywords :Young's modulus, Nanoindentation method, Films

References

- [1] Z. Fu et al., Journal of the European Ceramic Society 35 (2015) 2883–2893
- [2] H. Tanaka et al., Progress in Organic Coatings 170 (2022) 106941
- [3] Miyoshi et al., Koubunshi Ronbunshu 35 (1978) 125-129

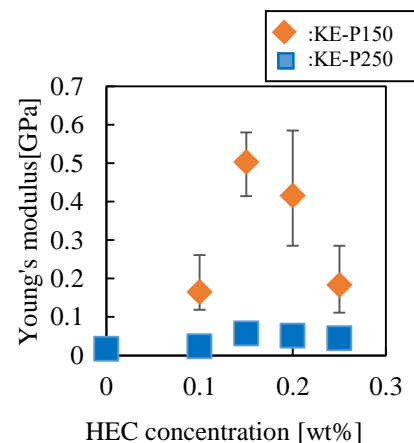


Fig. 1 Variations in elastic modulus of silica particle films with polymer concentrations at different particle diameters of 2.5 μm (square) and 1.5 μm (diamond)

Simulation study of the crystallinity on the colloidal film in drying process

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Abstract

We explore the drying process of mono-dispersed colloidal films via Brownian dynamics (BD) simulation [1]. For the target system, the effects of process variables such as drying and sedimentation speed on the microstructures of the colloidal film are carefully investigated. We describe the system in which the hard-sphere particles are dispersed in Newtonian liquid with particle volume fraction $\phi=0.1$. To understand the target system, we adopt the dimensionless number N_s which describes the relative strength of sedimentation to evaporation [2]. We carry out simulations for various N_s and analyze the structure of the colloidal film during drying. Firstly, the local particle volume fraction in drying films is explored. As N_s increases, sedimentation becomes dominant, and this leads to particle density increase near the substrate region. On the other hand, with a decrease of N_s , particle accumulation occurs near the liquid-gas interface. To validate the current simulation, we compare the results with a 1-dimensional equation [3,4] based on Wang and Brady's model. Results obtained by BD simulation and the model correspond to each other, and finally, we confirm their validity in predicting local particle concentration during drying and sedimentation. We also analyze the microstructure of colloidal films during drying. While a non-specific structure is observed until the intermediate drying stage, a dramatic structure change occurs in the final drying stage. Either crystalline (*e.g.* BCC, HCP) or non-crystalline structures are obtained and we derive the relationship between N_s and crystalline structure in the dried film.

Keywords: Colloidal particle, Brownian dynamics simulation, drying, sedimentation, crystallinity

References

- [1] J. H. Jeong, Y. K. Lee and K. H. Ahn, *Drying mechanism of monodisperse colloidal film: Evolution of normal stress and its correlation with microstructure*, AIChE J. 68(1), e17400 (2021).
- [2] C. M. Cardinal, Y. D. Jung, K. H. Ahn and L. F. Francis, *Drying Regime Maps for Particulate Coatings*, AIChE J. 56(11), 2769 – 2780 (2010).
- [3] M. Wang and J. F. Brady, *Microstructures and mechanics in the colloidal film drying process*, Soft Matter 13(44), 8156-8170 (2017).
- [4] A. F. Routh and W. B. Zimmerman, *Distribution of particles during solvent evaporation from films*, Chem. Eng. Sci. 59, 2961 – 2968 (2004).

Rheo-impedance behavior of inkjet inks during drying process

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Abstract

Pigment ink performs a good contour compared to dye ink, but tends to cause blockage at the inkjet nozzle. In order to avoid the blockage, the ink structure analysis while drying is a clue to grasp. Therefore, we evaluated the rheo-impedance behavior of a commercially available pigment-type inkjet ink (black, 75.8% water content) during the drying process. A disposable plate with a fixed drop of sample was mounted on the rheometer (MCR302e, Anton Paar), and dry air (70 cc/s) at a dew point of -40°C was supplied while the sample weight change and rheo-impedance measurement (strain 10%, angular frequency 10 rad/s, nonlinear region) were performed separately.

Fig. 1(a) shows the results of the drying experiment. The evaporation residual of the sample (W_t/W_0) showed three stages of change: an initial linearly decreasing the region I (constant rate period), followed by the region II (falling rate period), and the region III. The evaporation residual at the transition from region I to II and from region II to III were about 48% and 28%, respectively, independent of temperature. The evaporation rate during the constant rate period in the region I can be described as a zero-order reaction form, while the falling period in the region II can be described as a first-order reaction form [1]. Fig. 1(b) shows the change in the storage modulus G' as a function of the amount of evaporation residual. G' was zero for a while after the water in the sample began to evaporate, but then G' increased rapidly. The point at G' begins to increase rapidly coincides with the point of the transition from Region I to Region II. Fig. 1(c) shows the internal resistance R [2] calculated from the impedance measurement against the evaporation residual. R also increase rapidly as the evaporation progressed and the evaporation residual fell below 50%. The point of rapid increase in R coincided with the transition point from Region I to II, similar to the change in G' . That is, in the Region I, excess water from inside the bulk is easily supplied to the surface and evaporates independent of the water content. In the Region II, a concentration gradient of water in the bulk occurs with the formation of aggregated structures due to the pigment particles. As a result, the evaporation of water becomes proportional to the remaining water concentration, and we guess that water evaporation is suppressed.

Furthermore, in the Region III, G' tends to increase and R tends to decrease at higher drying temperatures, clearly indicating that there is a drying temperature dependence, suggesting that the aggregation structure of pigment particles formed differs depending on the drying conditions. This may be due to differences in the amount of the water trapped inside the aggregation structure.

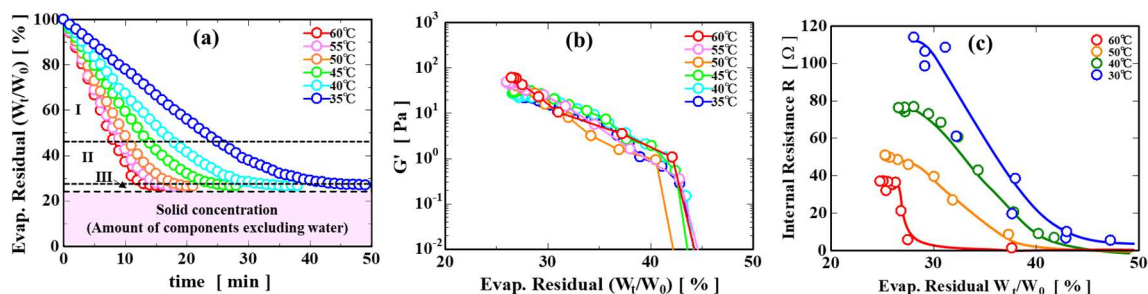


Figure 1. Changes in evaporation residue W_t/W_0 (a), storage modulus G' (b), and internal resistance R (c) as a result of water evaporation

Keywords: Rheo-impedance, viscoelasticity, drying process, inkjet ink, evaporation residual

References

- [1] T. Yoshida, *Drying by evaporation*. Shikizai. 40, 68-74 (1967).
- [2] Y. Yamagata, Y. Shimma, T. Ogura, K. Miyamoto, *Evaluation of phase inversion behavior of cleansing cream under shearing by rheo-impedance*. IFSCC Magazine, 26, 317-323 (2023)

Analysis of Mechanical Properties of PVDF-HFP Polymer Binders by Molecular Dynamics Simulation

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Abstract

The current lithium-ion battery (LIB) market is expanding rapidly. Binders are essential to maintaining the high capacity and longevity of batteries. Among them, Poly(vinylidene fluoride) (PVDF) binder is a representative organic binder that offers excellent electrochemical stability. To solve low adhesive force and weak mechanical strength of conventional PVDF binders, hexafluoropropylene (HFP) is added to improve these properties. However, the present poly(vinylidene fluoride-hexafluoropropylene) (PVDF-HFP) binders still show lower adhesive force than other polymeric binders, and therefore further research works are necessary.

In this study, we employ classical molecular dynamics (MD) simulations to investigate the structural properties of the PVDF-HFP copolymers. To create realistic disordered PVDF-HFP polymers, we develop a computational scheme that can randomly arrange the angles and sequences of the constituent polymer chains. By varying the ratio of randomly arranged PVDF-HFP copolymers to 0/100, 5/95, 10/90, 15/85, and 20/80, we build a solution model that mimics the HFP concentration of PVDF-HFP (0–20%, Sigma Aldrich) used in the actual experiments. N-methyl-2-pyrrolidone (NMP) used as solvents. To create a large-scale model, we utilize the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) and set parameters by using OPLS force field.

After creating the simulation model, NMP molecules are evaporated to produce a polymer film consisting only of PVDF-HFP polymers. Then we perform the adhesion analysis by applying forces to five polymer film models with different composition ratios in various conditions. Throughout these processes, we find the characteristic changes depending on the composition ratio. Finally, we will present the possible routes that can enhance adhesive properties of PVDF-HFP, which is a key requirement to the development of high performance binders.

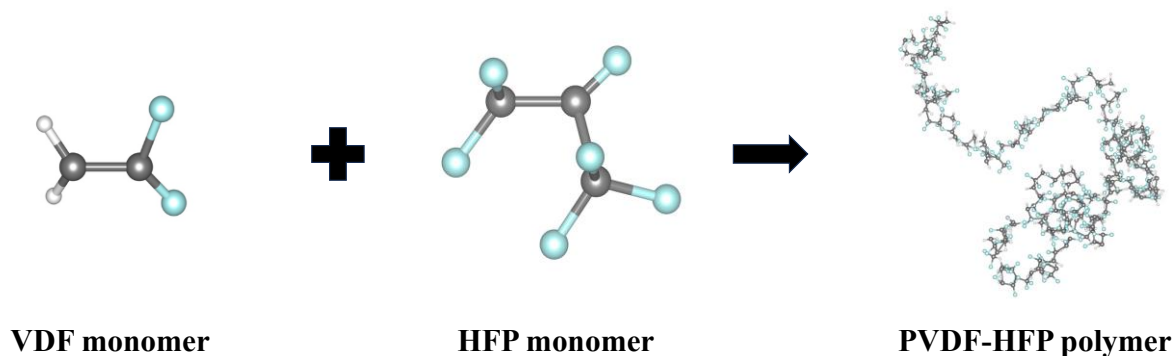


Figure 1. Picture of Random PVDF-HFP polymer

Keywords : Li-ion Battery, Polymer Binder, PVDF-HFP, Molecular Dynamics Simulation, LAMMPS

References

- [1] Gregorio, Jr., R., & Ueno, E. M. Effect of crystalline phase, orientation and temperature on the dielectric properties of poly (vinylidene fluoride). *Journal of Materials Science*, 34(18), 4489–4500
- [2] Maulana, A., Arkundato, A., Sutisna, & Trilaksana, H. (2020). Mechanical properties of Fe, Ni and Fe-Ni alloy: Strength and stiffness of materials using lammps molecular dynamics simulation. THE 2ND INTERNATIONAL CONFERENCE ON PHYSICAL INSTRUMENTATION AND ADVANCED MATERIALS 2019.
- [3] Vicente, Javier; Costa, P.; Lanceros-Mendez, S.; Abete, Jose Manuel; Iturrospe, Aitzol (2019). *Electromechanical Properties of PVDF-Based Polymers Reinforced with Nanocarboneous Fillers for Pressure Sensing Applications*. *Materials*, 12(21), 3545–. doi:10.3390/ma12213545

Decomposition mechanism of fluoro-ketone as C_3F_6O : alternative film etching gas

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Abstract

Global warming is one of the serious problems about the earth's environment and the biggest cause of global warming is CO_2 released into the atmosphere, which has increased in concentration in proportion to the development of the industry, but other greenhouse gases such as perfluorocarbons (PFCs) and hydrofluorocarbons (HFCs) have also been shown to have a much stronger greenhouse effect than carbon dioxide. [1]

Because hydrofluorocarbons (HFCs) have a high infrared absorbency and long atmospheric lifetimes. The Global Warming Potentials (GWPs) which shows the degree to which other greenhouse gases contribute to global warming based on the impact of carbon dioxide on global warming, is 1,000 to 10,000 times as high as that of CO_2 (whose GWP is 1). CHF_3 molecule which is the simplest molecule among HFCs gases has 11,700 GWP index. [1]

These HFCs gases are used in various device-fabrication processes in the semiconductor industry, CHF_3 is used in the etching process of SiO_2 films. Since semiconductors are an indispensable part of modern technology. it is time to discover alternative gases with a low GWP index that can be used in the etching process.

Therefore, C_3F_6O isomer, one of the several Precursor gas candidates of fluoro-ketone, will be investigated for several radical species that decomposed during the etching process compared to the reference etching gas CHF_3 , and will be calculation the energy of decomposition path by performing computation details of the quantum chemical calculations, Gaussian09. [2]

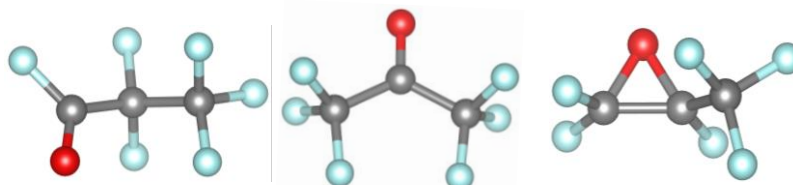


Figure 1. The isomer of C_3F_6O

Keywords: Etching gas, Density Functional Theory, Global Warming Potential, Plasma, Semiconductor

References

- [1] Okamoto, Y. Tomonari, M. "Ab initio calculations on reactions of CHF_3 with its fragments" J. Phys. Chem. A, 104(12), 2729-2733(2000).
- [2] Sinha, N. Choi, H. "Perfluoro-methyl-vinyl-ether as SF_6 alternative in insulation applications: A DFT study on the physiochemical properties and decomposition pathways" Comput Theor Chem, 1225, 114159(2023).

A Study on the Gas Decomposition Pathway Analysis for the Development of Fluorocarbon Film Deposition and Etching Process Using alternative Low-GWP Gas

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Abstract

As we progress towards a carbon-neutral society, there is a growing emphasis on utilizing semiconductor etching gases with reduced global warming potentials. This necessitates the exploration of alternative gases to replace conventional perfluorinated compounds (PFCs) currently employed in industrial processes. Oxygen-containing fluorocarbons have emerged as promising candidates for this role due to their lower propensity to generate environmental pollutants such as CO, CO₂, and COF₂. In this context, the potential utilization of compounds like Perfluoro-2-butanone and Perfluoro Tetrahydrofuran in ion plasma etching processes is of particular interest. These compounds offer the possibility of maintaining high process efficiency while minimizing environmental impact.

In this study, we theoretically investigate and compare the decomposition and recombination characteristics of the two isomers of C₄F₈O: Fluoro-ketone derivatives, Perfluoro-2-butanone, as well as the ring compound Perfluoro Tetrahydrofuran, using the Gaussian 16 software program. Additionally, our study aims to provide comprehensive insights into the decomposition pathways of neutral molecules, as well as ionization-induced decomposition pathways. By examining these aspects, we seek to offer a thorough understanding of the chemical transformations occurring during the decomposition and recombination processes of the investigated Fluoro-ketone as well as Perfluoro Tetrahydrofuran. This holistic approach allows for a detailed analysis of both neutral-state and ionization-induced reactions, shedding light on the intricate mechanisms governing the behavior of these compounds in plasma environments commonly encountered in semiconductor fabrication processes. By analyzing various reaction pathways, our research aims to contribute to the optimization of gas precursors, thereby enhancing semiconductor manufacturing technology to be more efficient and environmentally friendly.

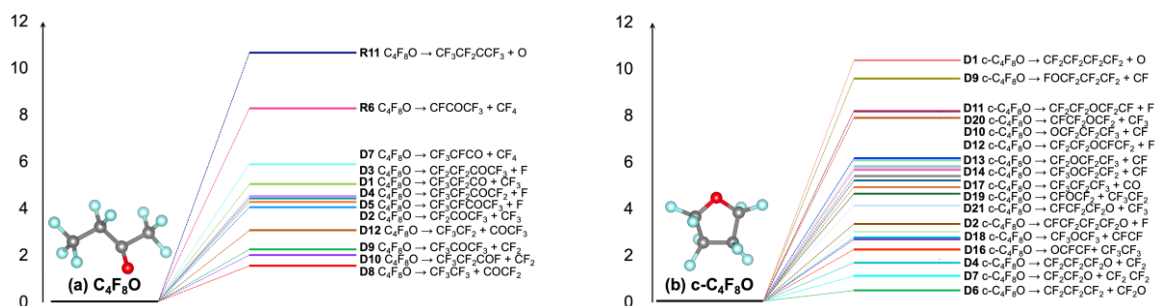


Figure 1. First stage decomposition pathway of Perfluoro-2-butanone and Perfluoro tetrahydrofuran

Keywords : Density functional theory, low-GWP, Etching gas, Carbon-neutral, Plasma