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Digital Twin Model of Paper−Aluminum Laminates for Sustainable Packaging

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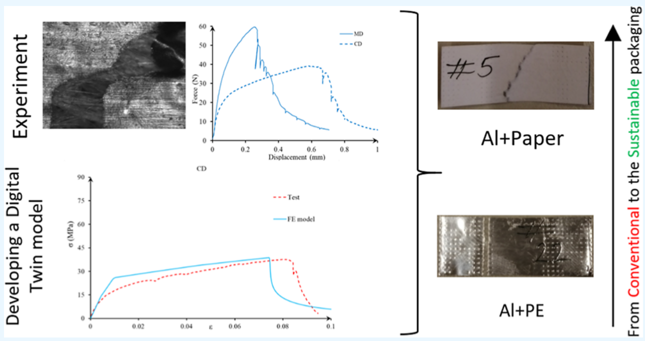
ABSTRACT: The proposed integrated experimental and simulation study focuses on the mechanical behavior and failure analysis of coupled paper−aluminum (paper−Al) laminates for sustainable packaging. The research employs an innovative experimental approach combining uniaxial loading with in situ visualization of sample deformation. The acquired experimental data are utilized to validate a simulation model, ensuring its accuracy and reliability. Parametric studies conducted through the finite element model further enhance our understanding of the mechanical behavior of the coupled laminates. Specifically, the study investigates microscopic mechanisms influencing the overall response of laminates in both the machine direction (MD) and the cross-machine direction (CD), presenting a comparative analysis with traditional aluminum−polyethylene (Al−PE) laminates, which is a prevalent choice in the packaging industry. The findings contribute to a better comprehension of key factors affecting the mechanical behavior of paper−Al laminates, enabling the design of more effective and sustainable solutions for the packaging industry. Results indicate the advantage of increasing the laminate thickness in the MD, demonstrating an enhanced strength. Conversely, the sensitivity of the thickness variation in the CD is found to be less pronounced. Additionally, our investigation highlights the substantial potential of paper-based materials as environmentally friendly alternatives, particularly in contrast to Al−PE laminates. Furthermore, integrating an innovative digital twin model, which combines experimental data and simulation, significantly advances our understanding and application of laminated in the context of paper packaging design.



1. INTRODUCTION

The packaging industry plays a pivotal role in ensuring products' integrity, safety, and presentation in modern life.[1] However, the industry impact on the environment has prompted a shift toward sustainable materials and design strategies.[2−4] In response to this, coupled laminates, which integrate multiple materials into a single composite structure, have gained attention for their unique combination of mechanical performance, barrier properties, and environmental sustainability.[5]

Traditionally, packaging materials relied on single-layer configurations, each one chosen for specific properties such as strength, flexibility, or barrier characteristics. For instance, aluminum is known for its excellent barrier properties against moisture, light, and oxygen, making it a popular choice for food packaging. However, it lacks the mechanical strength required for certain applications. On the other hand, materials like polyethylene (PE) offer good flexibility and strength but have poor barrier properties. While effective, these materials often presented inherent limitations, necessitating additional layers or coatings and contributing to increased material waste and environmental concerns. In contrast, coupled laminates represent a departure from this conventional approach by integrating two or more distinct materials into a single composite structure. This coupling is achieved through various methods, such as adhesive bonding, extrusion lamination, or coextrusion.[6] The result is a composite material that leverages the strengths of each constituent while mitigating their weaknesses.[7,8] This shift aligns with industry's commitment to sustainable practices. For instance, in a paper−aluminum (paper−Al) laminate, the paper layer provides the required mechanical strength and printability, while the aluminum layer provides the barrier properties.

In recent studies, it has been shown that the mechanical behavior of these laminates, particularly their fracture and delamination characteristics, can be effectively studied using experimental methods and simulation techniques.[1] These studies have provided valuable insights into the failure

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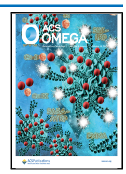

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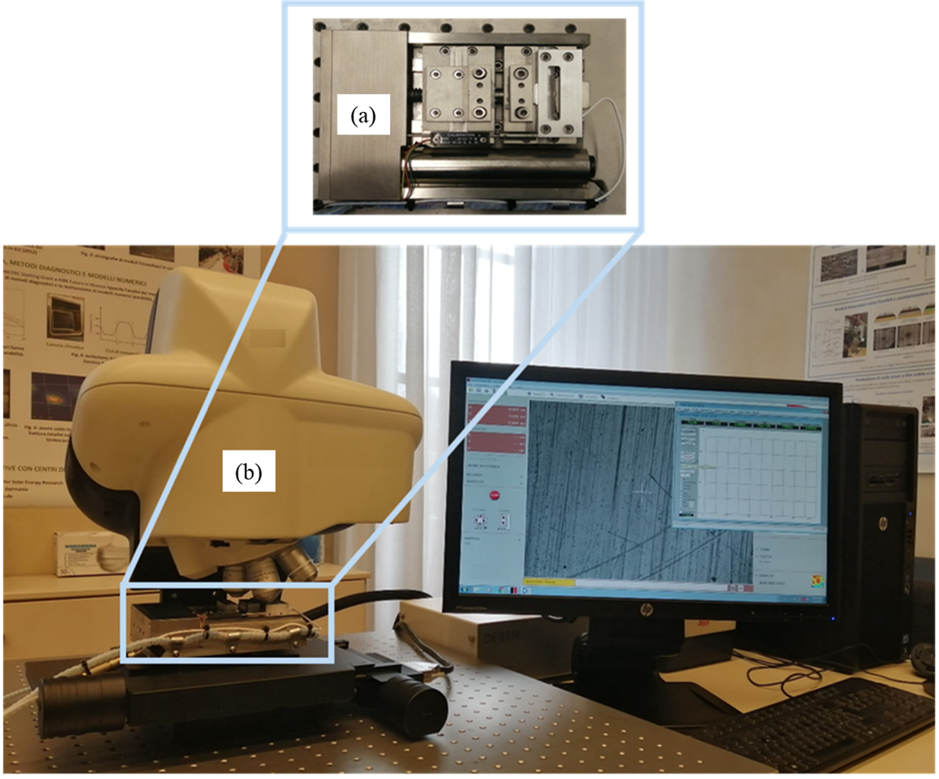

Figure 1. (a) DEBEN micromechanical tensile stage under (b) LEICA DCM3D confocal profilometer.

mechanisms of packaging materials, particularly in the context of package opening simulations.[9]

The drive toward sustainability and environmental consciousness has fueled innovation in the packaging industry, leading to the proliferation of coupled laminates featuring diverse material combinations. A notable choice among these is the aluminum−polyethylene (Al−PE) laminate, which is highly valued for its impermeability and flexibility. This combination proves to be robust, particularly in packaging for food and pharmaceuticals, offering moisture and oxygen barriers that extend shelf life.[9−12] However, the extensive use of plastic materials in Al−PE laminates raises environmental concerns, necessitating exploring eco-friendly alternatives.

In this context, our study focuses on the paper−Al laminate as an environmentally conscious solution, stemming from the need for greener alternatives due to environmental concerns associated with the prevalent use of PE. The dynamic outlook of sustainable packaging materials, including coupled laminates such as paper−Al and Al−PE laminates, emphasizes the industry commitment to addressing environmental concerns while meeting the functional demands of packaging. These material options provide opportunities to balance the performance and sustainability, aligning packaging practices with a more eco-conscious future. The motivation behind our research is to comprehensively understand the mechanical behavior and failure mechanisms of coupled laminates with a specific emphasis on paper−Al laminates. While the potential environmental benefits of paper−Al laminates are evident, their mechanical performance and limitations compared to those of Al−PE laminates necessitate accurate examination. This understanding is crucial for optimizing the design of packaging materials that are not only sustainable but also meet the strict demands of the industry.

In the present study, we employ an innovative experimental technique to investigate the micromechanical aspects governing the behavior of paper−Al laminates. Furthermore, by comparison of the mechanical behavior of the laminates with that of Al−PE laminates, their respective strength and weaknesses are analyzed. This investigation into the failure analysis and mechanical behavior of coupled laminates, specifically emphasizing paper−Al laminates, contributes significantly to the ongoing efforts to transform the packaging industry. By elucidating the microscopic mechanisms that underpin their performance, we aim to empower packaging engineers and designers with the knowledge needed to create more effective, sustainable, and environmentally friendly laminates for the future. This research not only addresses a critical aspect of packaging design but also paves the way for advancements in modeling and simulation through high-fidelity digital twin models, further propelling the industry toward a greener and more sustainable future.

2. MATERIALS AND METHODS

2.1. Experimental Testing. We implemented a novel experimental setup to conduct an in-depth investigation of the mechanical characteristics, fracture behavior, and damage mechanisms of coupled laminates. This setup featured a DEBEN micromechanical tensile stage positioned beneath a LEICA DCM3D confocal profilometer, as exemplified in Figure 1, to observe the evolution of damage throughout the tensile loading process. The equipment is available in the MUSAM-Lab of the IMT School for Advanced Studies Lucca. We selected a deliberately slow loading rate of 0.1 mm/min to enable the comprehensive capture of damage progression during loading, although different loading rates can be considered, as well.

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For this study, we selected two distinct coupled laminates: one composed of aluminum and paper and the other composed of aluminum and PE. The samples were 30 mm × 12.5 mm, with 10 mm of each side clamped securely, as illustrated schematically in Figure 2. Recognizing the potential for sample slippage in the grip during testing, we implemented a modification of our setup. To avoid any slippage of the sample in the grip, we adhered a paper on both sides of the sample. This modification provided additional friction at the contact points, effectively preventing the sample from slipping during the tests.

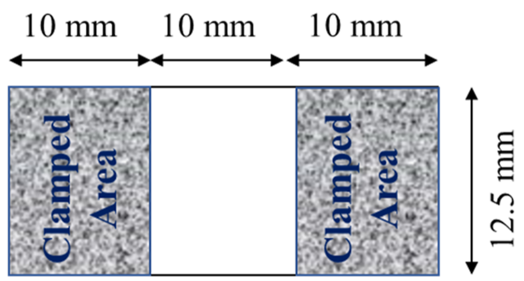

Figure 2. Schematic illustration of the sample dimension.

For illustrative purposes, we present a detailed analysis of the tensile behavior and damage evolution observed in a coupled laminate composed of aluminum and paper, specifically, in the MD. Figure 3 is a visual representation, effectively conveying essential insights into the material's response to the mechanical loading. This includes the force−displacement curve and the progression of damage observed in the loaded sample at various levels of elongation.

It is imperative to emphasize that throughout our parameter study, precise care was taken to ensure the reliability and robustness of our results. At least three individual samples were tested for each studied parameter to reduce the potential experimental uncertainties. The test results of the three similar samples were in good agreement (see Figure 4), indicating that our experimental setup and procedures were consistent and reliable. Therefore, within this study, we chose the data of one sample for our analysis. This decision was based on the observation that the test results of the three samples were closely aligned, suggesting that any one of them could be representative of the overall behavior.

These figures (Figures 1−3) depict essential components of our experimental setup and results, enhancing our clarity and understanding of our research methodology.

3. RESULTS AND DISCUSSION

3.1. Loading Rate Effect. To ensure the reliability of the microtensile test stage results, macrotensile tests using a universal testing machine available in the Center of Paper Quality of Lucense were also conducted. As previously mentioned, the microtensile test employed a loading rate of 0.1 mm/min, whereas for the macrotests, a rate of 10 mm/min

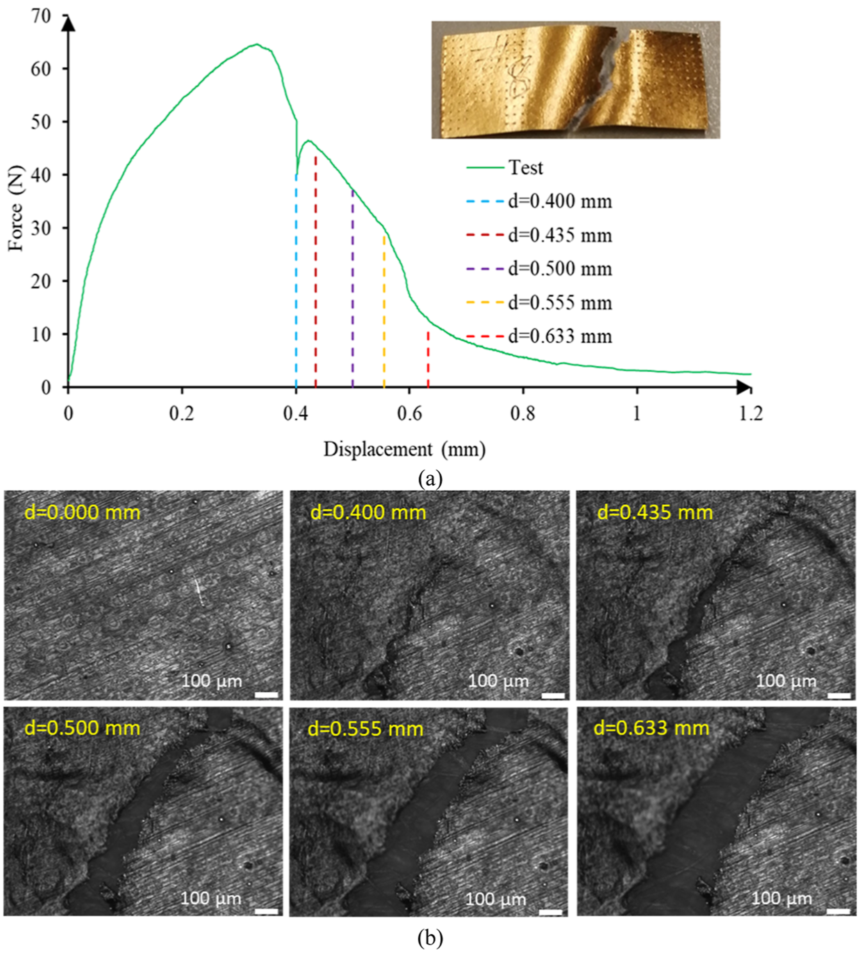

Figure 3. (a) Force−displacement and (b) damage evolution of the paper−Al laminate subjected to uniaxial tensile loading.

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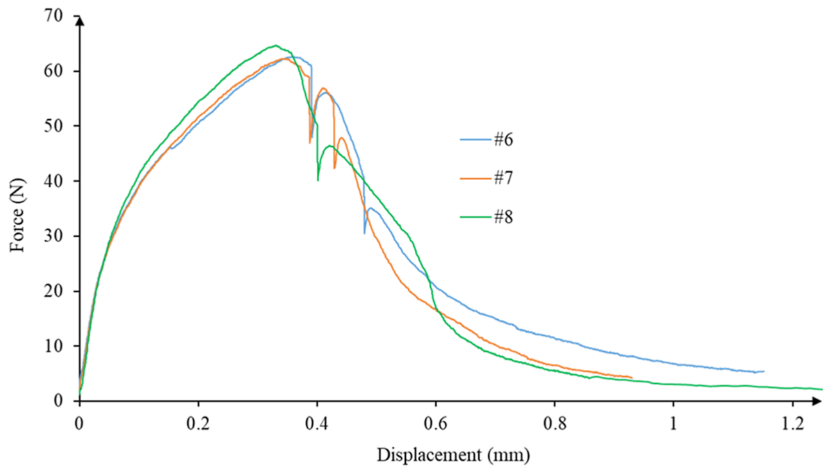

Figure 4. Tensile test results for three repeated experiments of coupled samples.

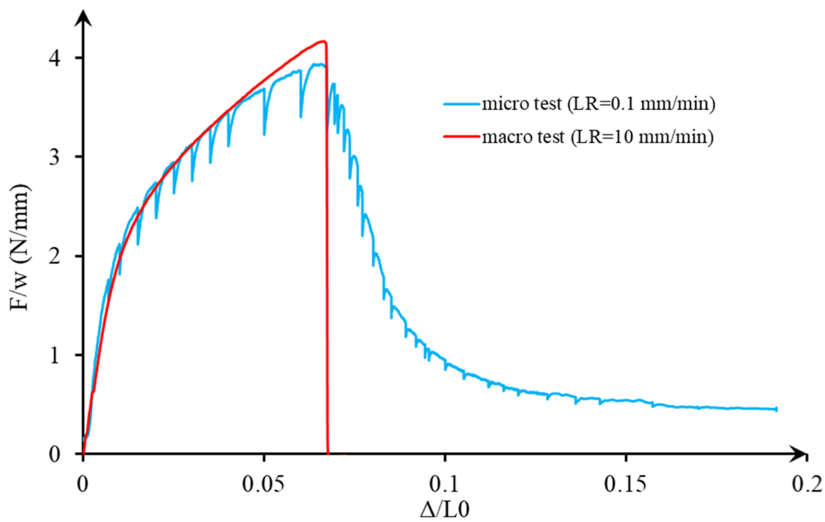

Figure 5. Tensile behavior of the samples: micro- vs macrotests.

was used. The corresponding results of paper−Al laminates are presented in Figure 5, demonstrating a good agreement between the two independent testing conditions and machines with a marginal effect of the loading rate for these materials. Notably, employing the microtensile test setup provides the advantage of capturing the postpeak behavior of the sample, specifically measuring the paper's contribution during the fracture process. It is important to mention that the load drops on the microtensile curve occur because the test has been temporarily paused to capture a photo of the sample, and a material relaxation takes place.

3.2. Material Anisotropy. This section explores how the loading direction with respect to the internal microstructural direction of the material caused by processing (MD or CD in the sequel) affects the tensile behavior of coupled laminates consisting of aluminum and paper.

In the manufacturing process of paper, the alignment of fibers predominantly occurs in the machine direction (MD), resulting in anisotropic mechanical properties. This anisotropy is reflected in the mechanical behavior of the paper−Al laminates. When the loading direction is aligned with the MD, the fibers' alignment direction, the laminate exhibits higher strength. This is because the fibers are well aligned to resist the applied load, resulting in a higher tensile strength and a more brittle behavior. This is also why we observe a zigzag pattern in the crack propagation in the MD, as the crack tends to follow the path of least resistance, which is between the fibers.

On the other hand, in the cross-machine direction (CD), the fibers are oriented perpendicularly to the loading direction. This results in a lower tensile strength, as the fibers are less effective at resisting the applied load. However, the laminate exhibits more ductile behavior and larger elongation in the CD. The fiber connections in the cracks of the CD laminate are a result of this fiber orientation. As the load is applied perpendicularly to the fiber direction, the fibers tend to pull out or debond from the matrix rather than break, leading to fiber bridging and a more tortuous crack path.

Figure 6 displays the respective samples' force−displacement curves and failure patterns. Notably, our observations reveal that initial damage occurs in the aluminum layer, regardless of the direction of loading, with respect to the MD and CD directions. Furthermore, when the loading direction is aligned with the MD, the striations within the aluminum layer tend to deflect the crack path, resulting in a more zigzag pattern and, consequently, a higher apparent strength than in the CD. In addition, due to the brittle nature and superior strength of the aluminum layer in the MD, coupled samples in this direction can withstand higher force before the onset of aluminum cracking. In contrast, when

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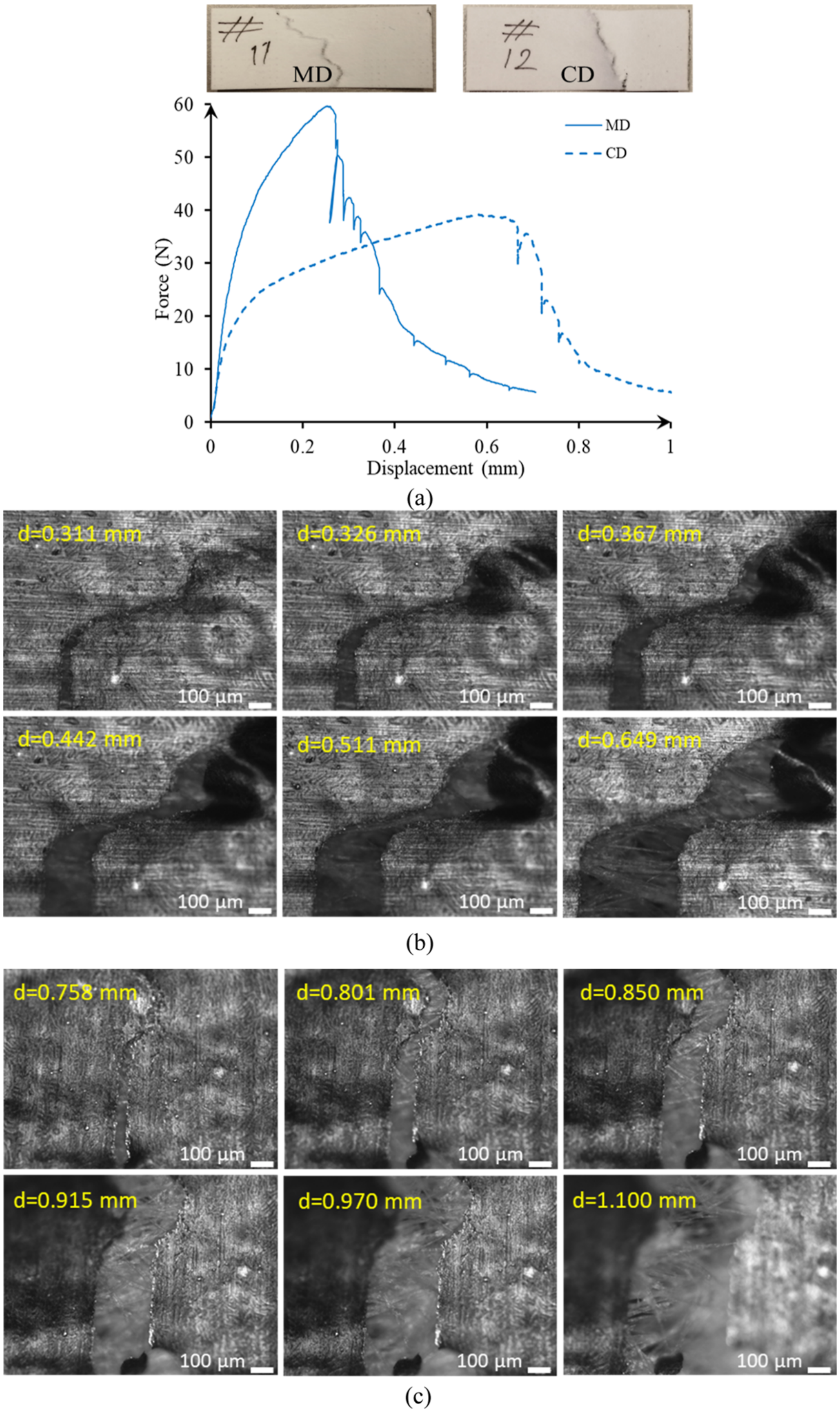

Figure 6. Tensile behavior of the coupled paper–Al laminate in the MD and CD: (a) force–displacement curve, failure pattern for (b) MD and (c) CD.

loading direction is applied in the CD, when cracking begins in the aluminum layer, the coupled sample experiences a lower force, preventing the paper layer's rapid tearing. Consequently, in the CD, the contribution of the fibers becomes more prominent, leading to a larger elongation and a more ductile behavior than in the MD.

3.3. Effect of Sample Thickness. To investigate the impact of sample thickness on tensile behavior, two cases with identical configurations and by variation of the thickness of the aluminum lamina are considered: one with 6.5 μm and the other with 12 μm. The corresponding force–displacement curves are shown in Figure 7. Results highlight that increasing laminate thickness enhances strength in both MD (solid lines) and CD (dashed lines). However, this increase in laminate thickness has a negligible influence on the final elongation of the CD.

3.4. Comparing Paper–Al and Al–PE-Coupled Laminates in Packaging. In the packaging industry, the prevailing choice for laminated materials often involves fusing aluminum layers with petroleum-based plastics, such as PE and polypropylene (PP). This conventional approach, while

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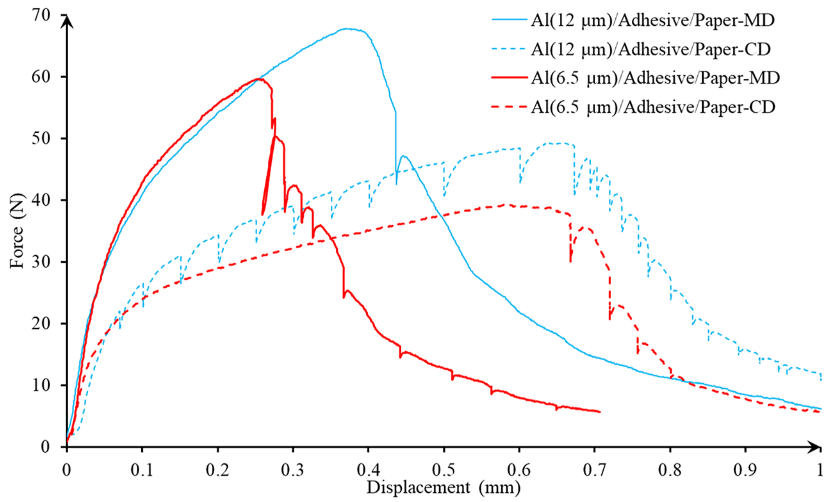

Figure 7. Force−displacement of coupled samples with different thicknesses.

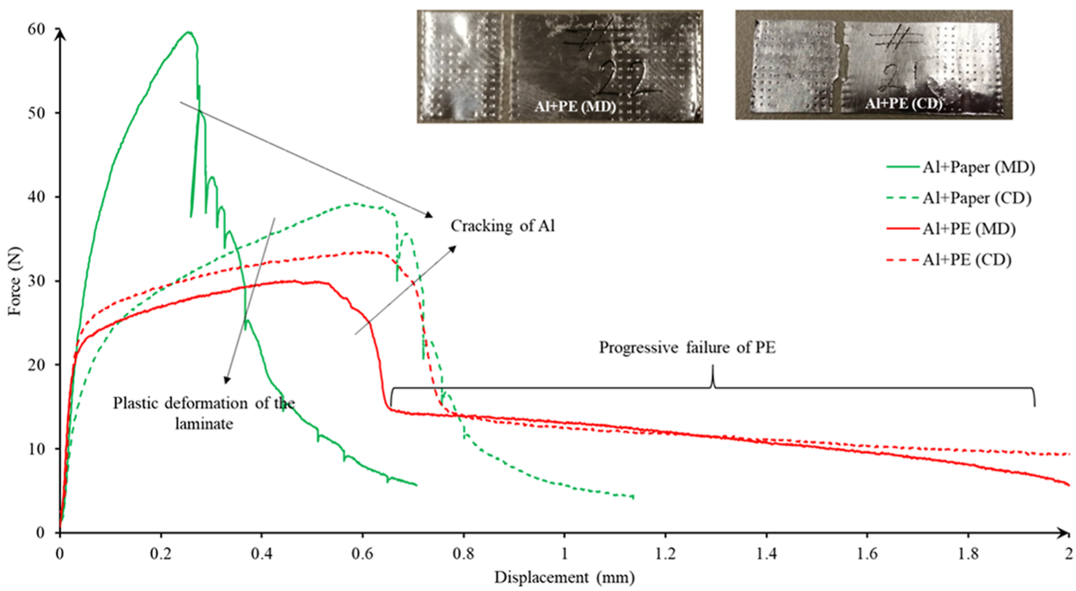

Figure 8. Comparative tensile behavior analysis of the paper−Al laminate and Al−PE-coupled laminate in packaging.

efficient, has raised pertinent environmental concerns. In response to these challenges, innovative solutions have emerged, seeking to not only preserve performance standards but also address the ecological footprint of packaging materials.

In this context, we initiate a comprehensive comparison between our sustainable alternative, comprising an aluminum and paper laminate, and the conventional laminate consisting of aluminum and PE. The conventional laminate has constituent thicknesses of 6−20 μm for aluminum and 15−50 μm for PE, while our sustainable solution uses paper with a weight of 60−120 g/m^2. The focus of this examination lies in the tensile behavior of the latter coupled laminate and the subsequent evaluation of damaged samples, as depicted in Figure 8. This performance is then set against the response of the paper−Al laminate.

Our observations disclose distinctive characteristics in the case of the aluminum−PE laminate. Notably, the failure pattern in both loading directions is manifested as perpendicular to the loading direction. Moreover, the force−displacement curve exhibits a trend similar to that in both directions. However, owing to the inherent properties of PE, the Al−PE laminate demonstrates superior elongation and a more gradual failure progression compared with the paper−Al laminate.

Figure 8 provides critical insight into the tensile behavior of the environmentally friendly solution (paper−Al) in the CD, showcasing remarkable similarity to the current industry standard (Al−PE) in packaging applications. Conversely, in the MD, the paper−Al laminate exhibits a more brittle behavior characterized by higher strength and reduced deformation at failure as compared to the Al−PE laminate. Hence, the eco-friendly solution would be optimal for applications requiring high strength and low ductility. This subtle comparison highlights the multifaceted nature of our eco-conscious packaging solution, offering a promising alternative in the quest for sustainable packaging materials.

3.5. Digital Twin Model. In this section, we thoroughly explore the computational aspects of our research, providing insights into the outcomes of our simulations. Our approach employs a 2D finite element model, implemented using Abaqus software, to replicate the microtensile test scenario. This model incorporates a clamped boundary condition with fixed displacement on one side, while the other side is subjected to controlled

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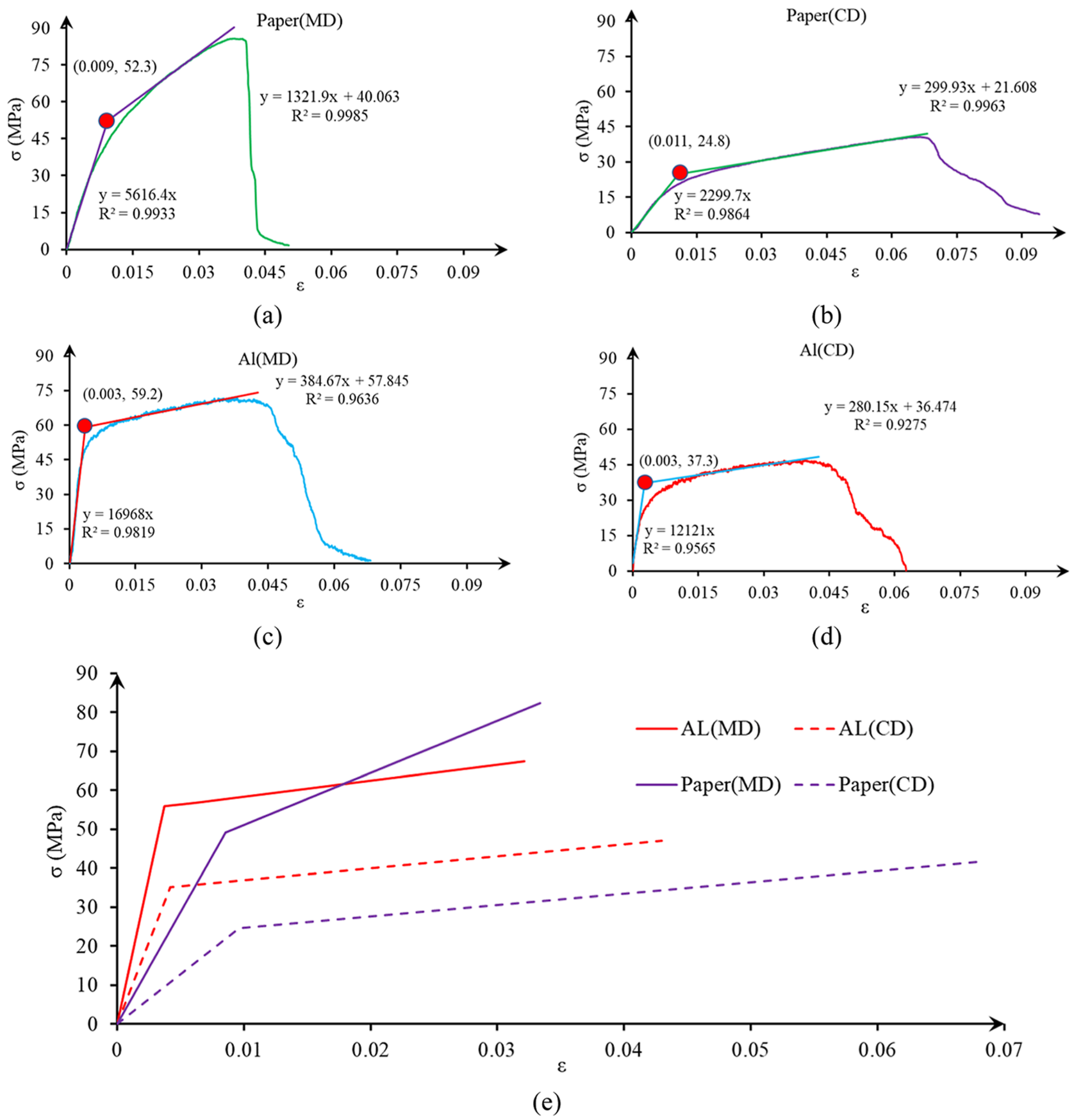

Figure 9. Bilinear elastic−plastic model derived from tensile testing of individual samples: (a) paper (MD), (b) paper (CD), (c) Al (MD), (d) Al (CD), and (e) for both materials in both directions in one plot.

displacement as a loading condition. The FE model uses a four-node bilinear plane stress quadrilateral (CPS4R) element type, which is well suited for modeling thin structures under plane stress conditions. The laminate is assembled by considering perfect bonding at the interface of the layers. This is achieved by using the "Tie" constraint option in Abaqus, which ensures that the nodes at the interface of the layers have the same displacement, effectively creating a perfect bond between the layers.

Building upon the tensile test data collected from individual paper and aluminum samples, we have formulated a robust bilinear elastic−plastic model to characterize the material behavior. This model, illustrated in Figure 9, with the properties listed in Table 1 plays a key role in our computational analysis, serving as a fundamental framework for comprehending how the coupled laminate materials respond to a variety of loading conditions. To consider the anisotropic behavior of the material, we used a Lamina type option for the elastic material properties of both layers (Al and paper). We input the elastic properties for both directions derived from the tensile test. This allows us to accurately capture the distinct mechanical behaviors in the MD and the CD.

Table 1. Material Properties of Paper and Aluminum in Both Directions

		E (MPa)	E_t (MPa)	υ_{12}	σ_y (MPa)	σ_u (MPa)
paper	MD	5739	1338	0.1	52.3	85.6
	CD	2558	293	0.1	24.8	33.8
Al	MD	15,045	410	0.32	59.2	68.4
	CD	8377	307	0.32	37.3	43.8

Through this model, we can gain a deeper understanding of the complex behaviors exhibited by these materials, providing valuable insights into their mechanical responses and structural integrity.

To verify the developed FE model, we turn to our experimental results as a robust benchmark for assessing the accuracy of our computational model. A detailed comparison between the finite element (FE) model and the test results in relation to a coupled laminate composed of paper and Al lamina, as depicted in Figure 10, demonstrates a high degree of

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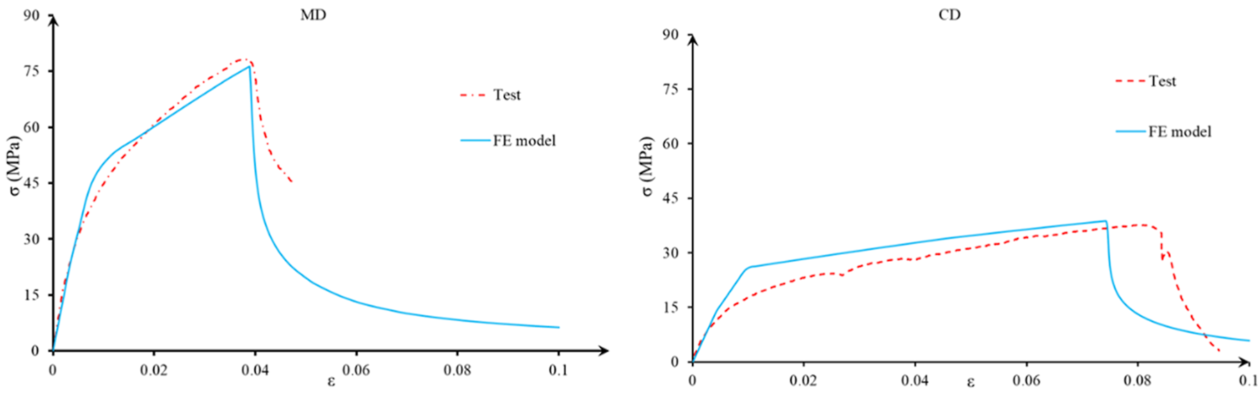

(a) MD *(b) CD*

Figure 10. Comparative analysis of FE model and experimental results concerning a coupled laminate composed of paper and Al lamina.

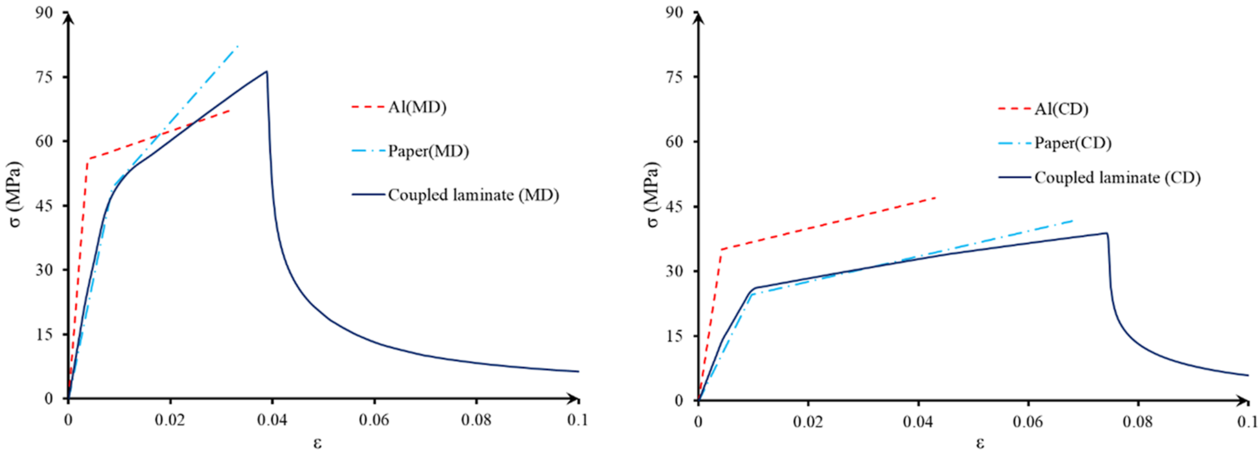

Figure 11. Tensile response of the coupled laminate vs individual aluminum and paper lamina.

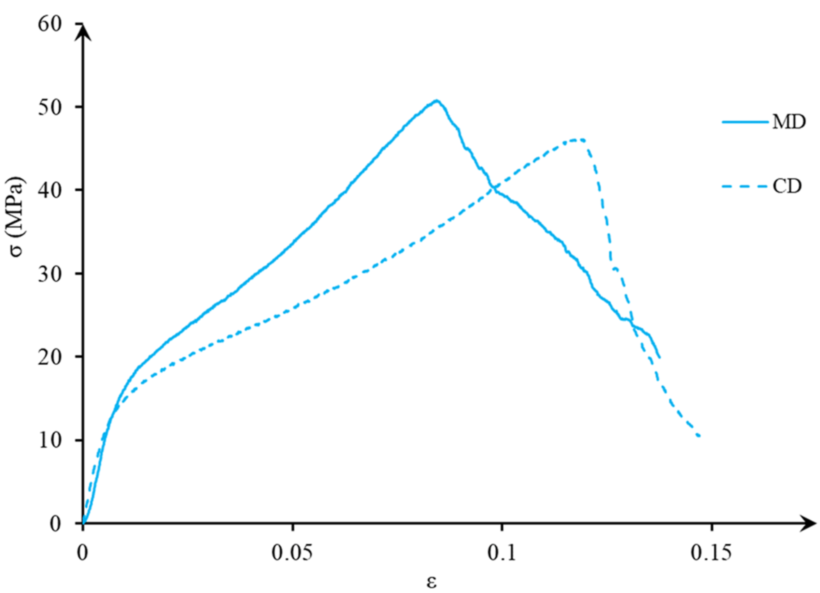

Figure 12. Tensile response of modified paper lamina.

consistency. This alignment signifies that our simulated model not only replicates the mechanical behavior of coupled laminates with great precision but also serves as a reliable predictor of their responses under various loading conditions.

3.6. Individual Constituent Contribution. In Figure 11, a comprehensive examination of the tensile behavior exhibited by the coupled laminate composed of paper and aluminum alongside the individual paper and aluminum lamina mechanical

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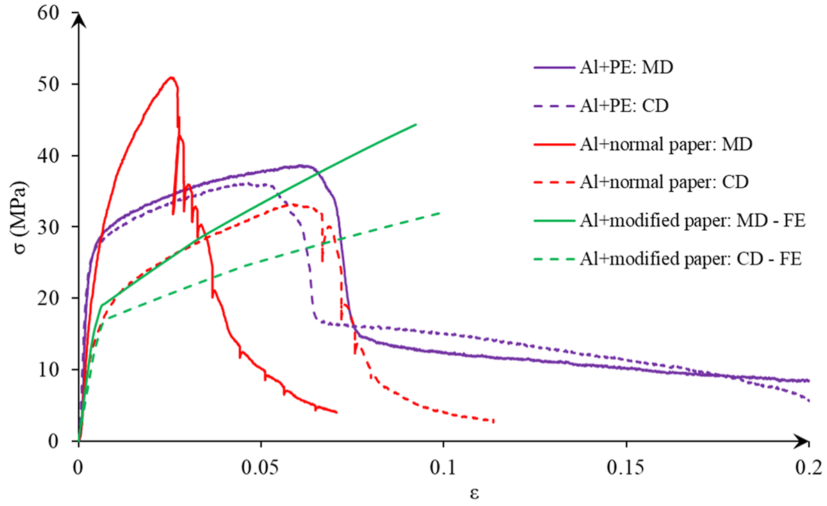

Figure 13. Tensile response comparison of the conventional coupled laminate and a sustainable alternative in both MD and CD.

responses is depicted. By closely inspecting the simulated results, a noteworthy inference arises: the mechanical response of the coupled laminate is primarily dictated by the behavior of the paper lamina. This observation highlights the key role played by the paper component in shaping the overall performance of the coupled material, offering valuable insights into its structural characteristics and response to mechanical loading. That means, paper plays a fundamental role in minimizing the difference between the mechanical responses in the CD and MD orientations. When chosen appropriately, paper allows for an almost isotropic overall response.

As mentioned earlier, the simulation results in Figure 11 show that the overall tensile behavior of the coupled laminate is mainly influenced by how the paper layer behaves. Looking at Figure 8, when comparing the tensile behaviors of the conventional coupled laminate, we notice significant similarities in both the MD and CD. This leads us to suggest that using a proper paper with comparable tensile behavior in both MD and CD, like the conventional Al + PE laminate to which we are comparing, can achieve the desired overall tensile behavior for the coupled laminate. This means our sustainable solution not only can behave like a conventional coupled laminate meeting the necessary performance standards but also being environmentally friendly.

To validate this concept, we used a modified paper, whose tensile test results for both MD and CD are shown in Figure 12. Subsequently, using our developed finite element (FE) model, we simulated the tensile behavior of a coupled laminate made of aluminum and modified paper. The results, shown in Figure 13, indicate that the tensile behavior of the coupled laminate with modified paper is better than that resulting from normal paper. Hence, by carefully choosing the right paper and adjusting the laminate thickness, we can achieve results very close to the conventional coupled laminate.

4. CONCLUSIONS

In the present integrated experimental and simulation study, our focus centered on investigating the mechanical behavior and failure analysis of paper−Al laminates, particularly in comparison with the current widely adopted Al−PE laminates in the packaging industry. The investigation explores the micromechanical aspects governing the behavior of paper−Al laminates in both the MD and the CD, providing crucial insights for the design of effective and sustainable laminates for the packaging industry.

The research methodology integrated innovative experimental techniques with a computational approach. The experimental setup involved a micromechanical tensile stage and in situ visualization to capture the evolution of damage during loading. This experimental data was then employed to validate a finite element simulation model, ensuring precision and reliability in our findings. Parametric studies conducted through the simulation model offered a deeper understanding of the mechanical behavior of paper−Al laminates.

Comparing the performance of the environmentally friendly paper−Al laminate with that of the conventional Al−PE laminate in packaging applications revealed promising characteristics. The Al−PE laminate, while demonstrating superior elongation due to the flexibility of PE, raised environmental concerns. The paper−Al laminate, on the other hand, exhibited more brittle behavior in MD, emphasizing higher strength and reduced elongation.

The analysis of individual constituents' contributions using the developed digital twin coupled model highlighted the significant role played by the paper layer in shaping the overall tensile behavior of coupled laminates. Having this finding in mind, a subsequent comparison with a sustainable alternative, employing a modified paper, indicated the feasibility of attaining outcomes closely resembling conventional coupled laminates (Al−PE) through careful material selection and thickness adjustment. This not only addresses the required performance standards but also, more importantly, aligns with environmental friendliness.

In conclusion, our study contributes to ongoing efforts for sustainability in the packaging industry by providing comprehensive insights into the mechanical behavior of paper−Al laminates. The environmentally conscious alternative demonstrates its potential as a sustainable solution, offering a balance between strength and flexibility. The findings empower packaging engineers and designers with valuable knowledge to create laminates that are not only effective but also aligned with the industry's commitment to environmental sustainability. As industry strives for greener and more sustainable practices, the research presented here marks a significant step forward in achieving that collective goal.

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Notes

The authors declare no competing financial interest.

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