Simulation-guided development concept for wood-based composites from sawmill byproducts

M. Lukacevic, M. Königsberger, G. Unsinn, M. Schwaighofer, V. Senk, L. Scolari, C. Hofbauer, N. Wahab, R. Ibadov, L. Zelaya-Lainez, S. Serna-Loaiza, T. Harter, M.Harasek, J. Füssl

Christian Doppler Laboratory for Next-Generation Wood-Based Biocomposite
Institute for Mechanics of Materials and Structures, Vienna University of Technology (TU Wien), Austria
Institute of Chemical, Environmental and Bioscience Engineering, Vienna University of Technology (TU Wien), Austria

TECHNISCHE UNIVERSITÄT WIEN
Vienna | Austria

WoodComp3D

Motivation and concept

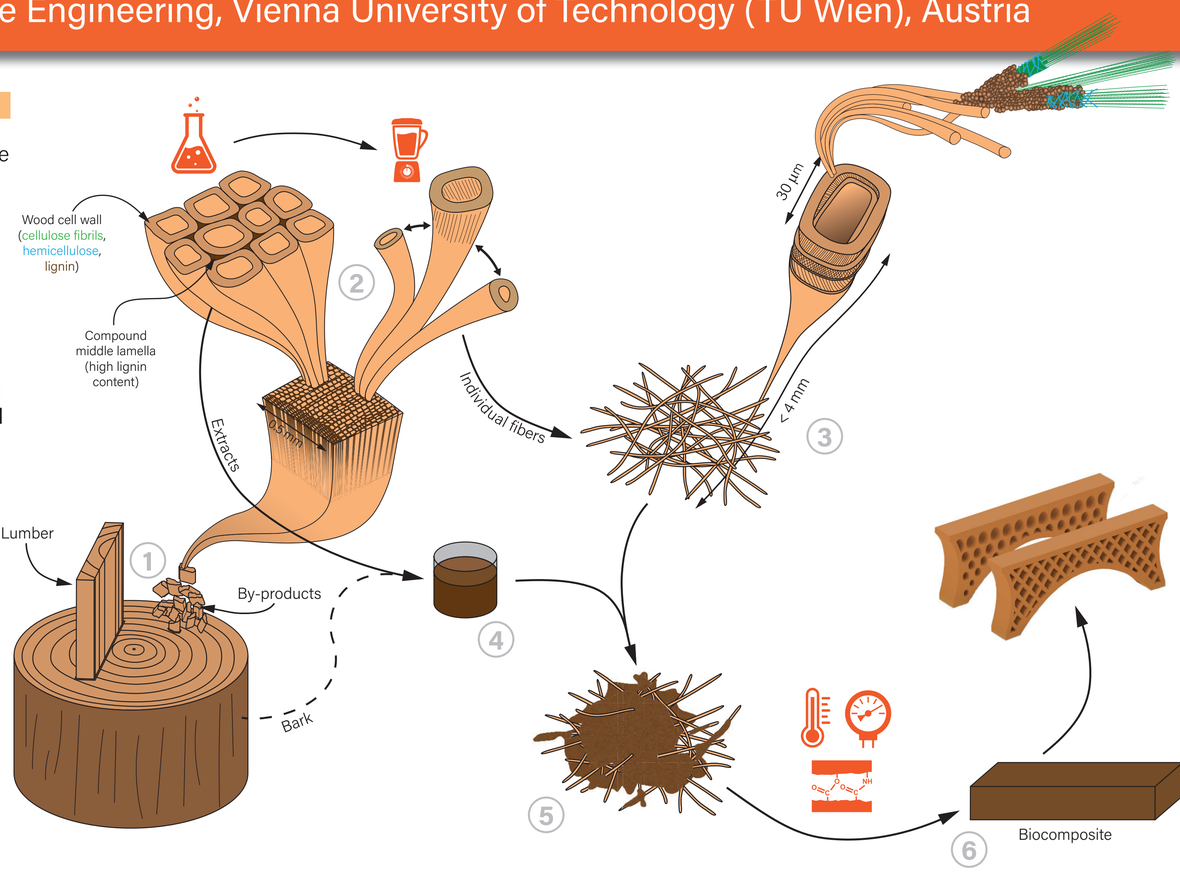
① During the production of lumber, a large proportion of by-products with different particle sizes is generated [1,2]. ② A combination of chemical and mechanical pretreatment is used to obtain ③ accessible and highly reactive fibers whose ligno-cellulosic composition can be tuned without destroying the inherent microstructure [3]. ④ The extracted components with high reactivity and cross-linking capabilities (also from underutilized parts of trees) are used as a binder in the ⑤ re-assembly stage [4]. There the formation of bonds leads to a ⑥ homogeneous and high-performant biocomposite material, which can be used in additive manufacturing processes.

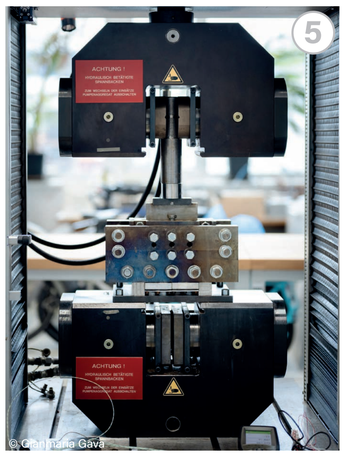
How can the mechanical behavior be described as a function of material characteristics at these different length scales, using multiscale modeling and simulation approaches?

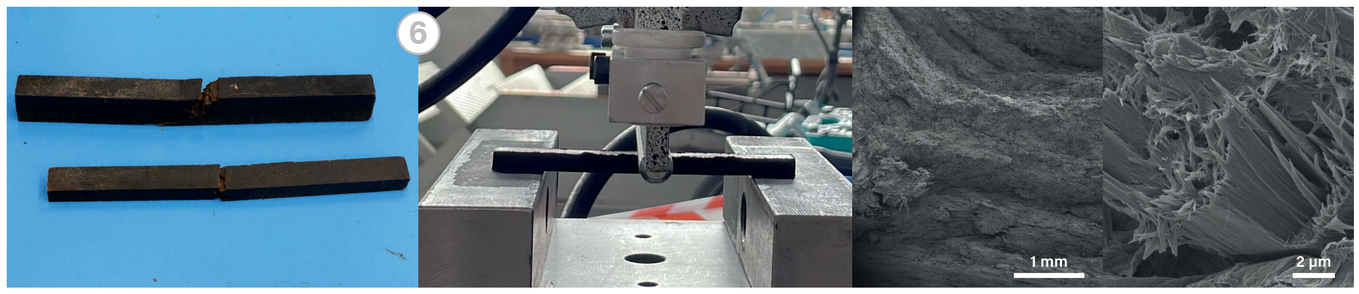
Nowadays, modeling concepts for biocomposites cannot describe all necessary mechanical processes on all relevant length scales. In contrast, often only basic models are used, which are supported by experimental campaigns.

In our modeling strategy, we combine fast analytical methods with very detailed non-linear finite-element-based simulations to describe the mechanical behavior of our new wood-based biocomposite on all length scales. This approach is complemented by the development of new identification experiments on multiple length scales.

With this approach and together with detailed analysis techniques, it is possible to specifically optimize a biocomposite material by providing rapid feedback on the material behavior. In this way, the decisive process parameters in the material development can be identified and optimized, and the material models can be used to study biocomposite-based structural elements before the actual production phase.



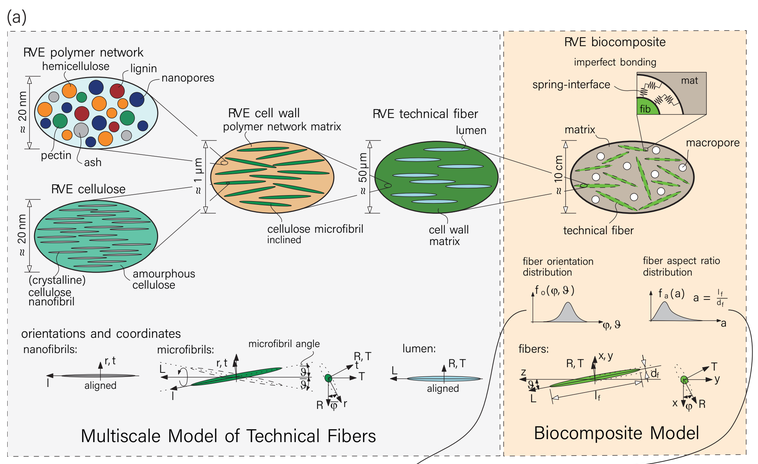




Modeling of mechanical behavior

We use two modeling strategies: continuum micromechanical models and detailed numerical models for nonlinear effects, like fiber-matrix interactions. For the former, we developed a model to predict plant fibers' stiffness and elastic limits [5]. Although the mechanical properties of these fibers vary widely, they all share basic components, with cellulose being the primary factor influencing mechanical behavior. Through continuum micromechanical multiscale modeling, the mechanical behavior of cellulose nanofibrils was upscaled to the technical fiber level (a). The predicted stiffness and elastic limits matched experimental values (b), validating the model and confirming that plant-specific physicochemical properties, such as microfibril angle and cellulose content, determine fiber performance. This model was further developed for plant-fiber-reinforced composites [6], including a spring-interface model for quantifying the compliance of the fiber-matrix connection and the ability to model any orientation and length ratio distributions, and allowing for various parameter studies (c).

In the numerical models (d), building upon models previously developed for wood [7,8], we study fiber-matrix interactions, modeling all possible failure mechanisms: matrix, interface, and fiber failure. We also explored the phase-field method [9] to improve the stability of nonlinear matrix behavior analysis. Representative volume elements for fiber-reinforced composites were developed to efficiently predict larger structures' mechanical behavior. The model was validated through comparison with existing tensile test data, with sensitivity analyses emphasizing the importance of matrix-fiber interface parameters. Due to the computational intensity, we aim to develop a multiscale approach that integrates the numerical model with the analytical micromechanics-based homogenization, e.g., by employing so-called deep material network models.



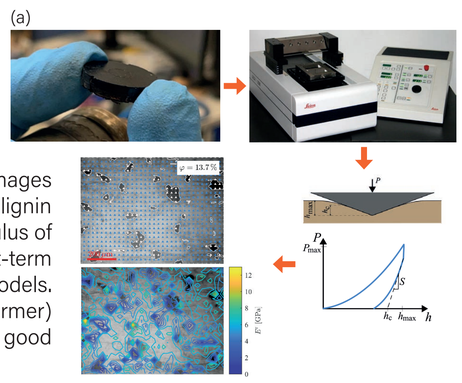
$$C_{hom} = \sum_{i=1}^{N} f_i \int_0^{\infty} f_a(a) \int_0^{2\pi} \int_0^{\pi} f_o(\vartheta,\varphi)\, C_i(\vartheta,\varphi) : A_i(\vartheta,\varphi;a) \sin\vartheta \, d\vartheta \, d\varphi \, da$$

Phase volume fraction — Phase stiffness — Concentration tensor

Mechanical characterization

To obtain the models' input properties and to validate them, various mechanical characterization experiments are needed. Macroscopic ones of the biocomposite itself, e.g., three-point bending tests ⑥, are not sufficient, but analyses of the resulting fracture surfaces by SEM already showed the contribution of the fibers to the strength of the biocomposite (MOR > 140 MPa).

(a) The stiffness and viscoelastic properties of hot-pressed lignins were studied using nanoindentation of polished specimens [10]. A statistical and microstructure-guided evaluation using microscopy images allowed determining reliable properties of porous lignin. The desired mechanical properties of pure lignin were back-calculated using a continuum micromechanics model, indicating an intrinsic elastic modulus of approximately 7 GPa [11] and showing that lignin is a viscoelastic material with a pronounced short-term relaxation behavior during tests [12]. (b) Single-fiber tests are used to further validate the multiscale models. (c) Various lap-shear and tensile tests with veneers or specially produced papers (dynamic sheet former) have already been investigated, in which all production steps can be replicated and thus provide a good basis for comparison with and further development of the biocomposite material.



References

[1] K. Lan, S. S. Kelley, P. Nepal, Y. Yao, Environ. Res. Lett. 2020, 15, 124036.
[2] Austrian Energy Agency, "Wood flows in Austria," available at https://www.klimaaktiv.at/erneuerbare/energieholz/holzstr_oesterr.html, 2020.
[3] X. Yang, F. Berthold, L. A. Berglund, Biomacromolecules 2018, 19, 3020.
[4] B. Jiang, C. Chen, Z. Liang, S. He, Y. Kuang, J. Song, R. Mi, G. Chen, M. Jiao, L. Hu, Advanced Functional Materials 2020, 30, 1906307.
[5] M. Königsberger, M. Lukacevic, J. Füssl, Mater Struct 2023, 56, 13.
[6] M. Königsberger, V. Senk, M. Lukacevic, M. Wimmer, J. Füssl, Composites Part B: Engineering 2024, 281, 111571.
[7] S. Pech, M. Lukacevic, J. Füssl, Finite Elements in Analysis and Design 2021, 190, 103531.
[8] M. Lukacevic, W. Lederer, J. Füssl, Engineering Fracture Mechanics 2017, 176, 83.
[9] S. Pech, M. Lukacevic, J. Füssl, Engineering Fracture Mechanics 2022, 271, 108591.
[10] L. Zelaya-Lainez, G. Balduzzi, O. Lahayne, M. Lukacevic, C. Hellmich, J. Füssl, Materials Today: Proceedings 2023, 93, 662.
[11] M. Schwaighofer, L. Zelaya-Lainez, M. Königsberger, M. Lukacevic, S. Serna-Loaiza, M. Harasek, O. Lahayne, V. Senk, J. Füssl, Materials & Design 2023, 111765.
[12] M. Schwaighofer, M. Königsberger, L. Zelaya-Lainez, M. Lukacevic, S. Serna-Loaiza, M. Harasek, F. Zikeli, A. Friedl, J. Füssl, Mechanics of Materials 2024, 188, 104864.

Acknowledgments

The financial support by the Austrian Federal Ministry of Labour and Economy, the National Foundation for Research, Technology and Development and the Christian Doppler Research Association is gratefully acknowledged. Furthermore, the authors would also like to express their gratitude to the CD laboratory company partner HS Timber for their financial support.

HS TIMBER GROUP

Christian Doppler Forschungsgesellschaft