HARNESSING MACHINE LEARNING FOR ACCURATE STRESS-STRAIN CURVE PREDICTION

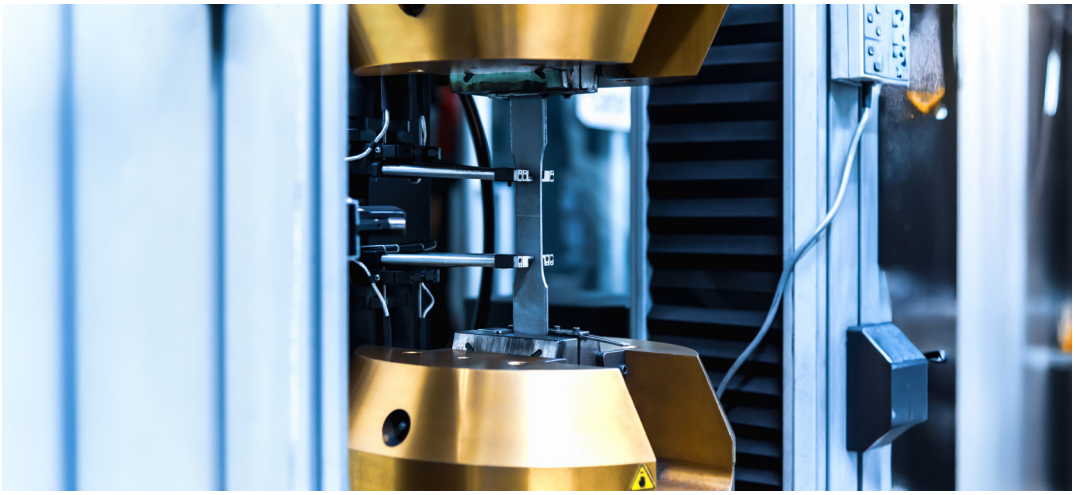
The integration of machine learning techniques into material science has revolutionized the way we analyze and explore material behavior. Predicting stress-strain curves is critical for quickly understanding a material's mechanical properties under different conditions. By tapping into datasets and innovative modeling techniques, we can make more accurate predictions of different material configurations virtually and narrow down the selection to the most suitable candidates for physical testing. In this technical document, we'll explore the challenges a team might face, Altair's solution, and the methodology behind it.

The Challenge

Choosing the right material for your application can be a lengthy and complex process. After narrowing down potential options, testing is required to ensure the material meets the necessary specifications. This often involves multiple rounds of testing, since performance can vary depending on conditions. Moreover, the time between material selection, ordering, and testing can span several weeks, and unexpected issues during testing can also add delays. This all slows progress and makes the decision-making process even more challenging.

Predicting stress-strain curves is crucial for three key groups involved in materials: material scientists, designers and engineers, and material producers and distributors. For material scientists, predicting stress-strain curves helps design new materials with specific mechanical properties, ensuring they meet performance standards. Designers and engineers rely on this data to select the best materials for their projects, ensuring optimal performance and safety under stress. Material producers and distributors benefit by having access to detailed material behavior information, which helps them market and sell materials to potential customers.

By predicting material performance, we can slash the number of options that require further testing and evaluation. This approach allows teams to focus on the most promising candidates, and ultimately streamlines material selection, development, and sales processes.



Our Solution

Reliable material data is the foundation of high-quality predictions. Ideally, this data has already been consolidated, validated, and structured. When teams need to do this, Altair® Monarch®—the industry's fastest, most user-friendly tool for cleaning and preparing unstructured data—proves invaluable. In tandem with Monarch, the Altair® Material Data Center™ empowers organizations to securely store and manage materials knowledge in their private database with complete traceability throughout the entire data life cycle.

To ensure accurate predictions, it's crucial to leverage all relevant data at the time of forecasting. For example, in the case of polymers, this typically includes data such as the base polymer, fillers, filler content, density, and results from simple impact tests. Even basic data of this kind can provide valuable insights and support the generation of accurate predictions. Plastic manufacturers may have access to more detailed information, such as impact modifiers and flame retardants. Including this data can further refine the machine learning model, improving its predictive capabilities.

With a more defined use case, the model can offer greater precision. For instance, if a material is tested at room temperature, the model can more accurately predict its behavior at other temperatures, improving the reliability of forecasts.

The Methodology

This innovative data pipeline integrates material science knowledge at various stages to create accurate, data-driven material behavior predictions. Initially, material science expertise is used to categorize materials hierarchically. This classification includes grouping materials by type – such as thermoplastics, elastomers, or thermosets – and determining whether they're amorphous or semi-crystalline. This classification helps structure the data in a meaningful way for further analysis and to leverage similarities between materials groups.

Next, physics-based formulas are applied to fit multipoint data such as stress-strain curves or creep curves to create a consistent step size for the curves. Each step is then used to generate a prediction, ensuring the model accounts for the full spectrum of material behavior. The machine learning algorithm also incorporates known material science constraints into its learning function. These engineering principles are encoded into the model, ensuring predictions are aligned with established material behaviors and real-world expectations. This pipeline is implemented in the Altair® RapidMiner® data analytics and artificial intelligence (AI) platform, making it easy for anyone to train predictive models using their own data. The platform's user-friendly interface enables seamless training and customization of the model based on specific datasets.

Finally, the prediction results are made easily accessible to designers, material data scientists, or simulation engineers through the Material Data Center database interfaces. Users can quickly compare and search for relevant data and export simulation-ready material cards for AI-generated materials, with users being informed of which data was AI-generated.

Conclusion

Altair's prediction pipeline offers a powerful solution for obtaining rapid, accurate results driven by valuable use cases and robust data. By combining material science knowledge with machine learning expertise, the pipeline ensures high-quality predictions. The results are easily accessible to users, facilitating seamless integration into their workflows. Altair provides direct integration with modeling and visualization tools such as Altair® HyperMesh®. Integration with third-party product lifecycle management (PLM) applications is supported through APIs. Additionally, Altair RapidMiner's no-code environment makes it simple to adapt and customize models, empowering users to tailor the system to their specific needs without requiring extensive technical expertise. Together, Altair RapidMiner and Material Data Center is a powerful solution that helps organizations maximize the potential of data and drive next-level innovation.

To learn more, please visit altair.com/altair-rapidminer