UTILIZING TECHNOLOGY FOR RATIONAL MATERIAL SELECTION

We start this piece with a key question: How would you choose a material to fulfil a product need? By the end of the article, we will have introduced two key concepts in material selection with one focused on a methodology that can aid product development today and another that stems from the emerging field of artificial intelligence (AI).

The good news is that there are lots of materials available for product development, from metals and ceramics to polymers, each with their own unique set of properties. However, it is completely reasonable that material selection can be one of the most daunting tasks - there are, seemingly, infinite options to choose from. The biggest risk is sticking with what you know or materials you have used in the past which could mean missing out on a competitive advantage. Worse still, when materials fail or underperform, the results can be catastrophic, leading to delays in production, market adoption or even fines from law suits and regulatory bodies. A good example is the story of the S.S. Schenectady built during World War Two. There is no doubt that the shipbuilding company picked materials based on key requirements. However, the ship's hull almost fractured in half due to the ductile-to-brittle transition of low-grade steel exposed to frigid waters. This signifies that it is not just picking the right material for the right application but understanding the range of constraints that the material will face during use.

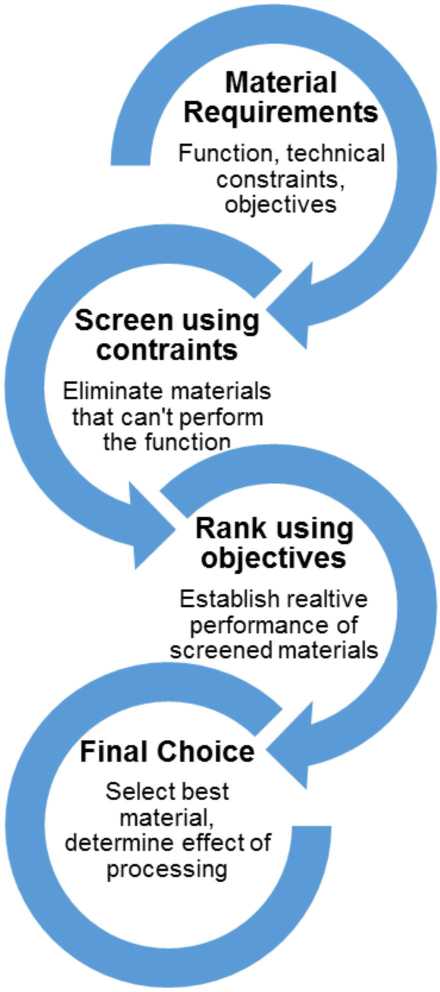

Figure 1. Rational material selection process

Material selection is full of compromises and tradeoffs that can make the process more difficult, however the rational approach, as shown in Fig 1., can make the task less daunting while drastically decreasing the time needed for initial screening. Rational material selection starts by identifying the function of the component being designed, technical constraints that need to be maximized or minimized and the objectives that must be met.

A simple example is a beam supporting a specific load in flexure with the objective of finding the lightest and/or cheapest materials. Subsequently, materials that cannot perform the function, because their flexural strength is below a specified level of constraint, can be screened or eliminated and remaining candidates can be ranked based on the objectives, i.e. low density or cost. Assurances can be made through the use of a material 'index' which is the combination of properties that maximize those aspects of component performance. With the aid of computer software and materials databases, the entire process can be performed quickly and visually in a meaningful way. It is important to emphasize that a rational material selection process does not eliminate the need for materials characterization and product validation, however, as noted above, the initial screening can certainly speed up the entire process. Once materials have been selected, optimizing the processing window of the selected material, and understanding how the two are unified in the design and function of the product, is the ultimate key to success.

While the rational approach is the effective methodology to select materials, industry is constantly evolving. We live in a data rich world that is driven by our ability to generate, store and transfer data over large distances primarily through the internet which means we are in touch with our environment and what is occurring around us more than ever before. AI is at the forefront of this data revolution with its ability to capture, organize and find patterns in masses of chaotic strings of numbers and letters that can make automation more efficient, protect us from fraud and understand our interests or spending habits. Machine Learning (ML) is a subset of AI and as a science is not new, but ML is gaining fresh momentum in materials science and chemistry. ML is an iterative process based on sequential learning to develop predictive models using algorithms that identify patterns in historical data. ML is analogous to the way that humans actively learn from known facts or past events but at significantly faster speeds afforded by today's computing power. Thus, ML promises to guide and reduce the product development timeframe by limiting the number of experiments needed to develop new materials with desirable properties. A vital recognition is that ML does not displace the need for scientists and engineers. Rather, expert domain knowledge of materials, physics, and chemistry is essential to decide which relationships are worth exploring to enhance the accuracy of the predictive models.

While ML is in a strong position to rapidly transform the way that new materials and technologies are developed or optimized, it is weighed against more familiar and widely used techniques. For example: statistical modelling, that establishes relationships between variables; and material indices, that contain groups of material properties as described in the rational material selection example above. Each method shares a common goal of predicting an outcome. The challenge, therefore for materials scientists and engineers, is choosing between each technique or understanding when one technique may be more beneficial over another.

It is clear that the promise of ML, to speed up the development and optimization of new materials, has captured the attention of industry. Numerous companies are using this technique to develop advanced materials, optimize processes and even detect failures in images or time-series data collected directly from the line. However, many companies lie on a broad spectrum of curiosity and familiarity with ML and a key question for most is whether ML can do better or work in concert with other methodologies. Regardless, for scientists and engineers to stay relevant in an ever changing, data-driven world, it is important to understand the benefits of ML and its home amongst conventional techniques.

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