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MATERIAL SELECTION USING LARGE LANGUAGE MODELS

Yash Patawari Jain†*
Dept. of Mechanical Engineering
Carnegie Mellon University
Pittsburgh, PA, USA
ypatawar@andrew.cmu.edu

Daniele Grandi†
Autodesk Research
San Francisco, CA, USA
daniele.grandi@autodesk.com

Allin Groom
Autodesk Research
London, UK
allin.groom@autodesk.com

Brandon Cramer
Autodesk Research
Boston, MA, USA
brandon.stewart.cramer@autodesk.com

Christopher McComb*
Dept. of Mechanical Engineering
Carnegie Mellon University
Pittsburgh, PA, USA
ccm@cmu.edu

ABSTRACT

The task of material selection plays a pivotal role in a large number of industries, from manufacturing to construction. Material selection is usually carried out after several cycles of conceptual design, during which designers iteratively refine the design solution and the intended manufacturing approach. In design research, material selection is typically treated as an optimization problem with one correct answer, and restricted to specific types of objects or design functions. In this work, we instead treat materials selection as a problem with multiple answers with varying feasibility. We collect a dataset of experts' material preferences for nine material categories across 16 diverse design scenarios, and report some trends in the data.

Recent advancements in the natural language processing field around transformer-based architectures, leading to the development of a multitude of pre-trained Large Language Models (LLMs) capable of understanding human language and exhibiting reasoning behaviors, raise some questions about the potential use of this technology for automating the material selection, especially during early the early conceptual design phase. In this work, we identify the degree to which material recommendations provided by an LLM align with those of expert human designers. The results underscore the potential of LLMs to inform material selection.

1. INTRODUCTION

The process of material selection is critical across a wide variety of industries, ranging from manufacturing to construction. It involves making informed decisions about the materials used in various products, structures, and systems. Traditionally, material selection occurs after iterative design cycles, where design modifications and manufacturing methods are refined. However, this approach often neglects the crucial role that materials may play in shaping the performance, cost, and sustainability of the final product.

Historically, material selection has often followed a 'manufacturing first' approach in which designers and engineers tend to prioritize manufacturing feasibility over material suitability. Consequently, this bias can lead to suboptimal material choices, impacting product performance, durability, and overall quality. Not all designers possess extensive material expertise. Many lack the necessary knowledge to evaluate material properties, compatibility, and trade-offs effectively. Bridging this knowledge gap is essential for informed decision-making. Material selection decisions made early in the design process significantly influence downstream activities, so ensuring that these decisions align with the project goals and constraints is crucial.

The recent development of large language models (LLMs) in the machine learning domain [1–6] presents a novel opportunity to streamline the material selection process in the mechanical design domain. LLMs are a type of model capable of generating human language. They have been successfully employed in various domains, including design [7–13], where they have demonstrated the ability to generate creative and novel visual and

†Joint first authors
*Corresponding author: ccm@cmu.edu
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textual design solutions.

In this research project, our primary objective is to integrate LLMs into the material selection workflow, with a focus on overcoming the limitations of the manufacturing-first approach and empowering designers with data-driven decision-making tools. Specifically, we aim to address the following key objectives:

1. Streamline Decision-Making: LLMs provide an innovative avenue for automating and accelerating material selection. Their ability to analyze vast amounts of textual data, scientific literature, and engineering specifications allows for more efficient decision-making.

2. Address the Manufacturing-First Issue: We seek to shift the paradigm by emphasizing material suitability alongside manufacturing feasibility. LLMs can assist in identifying materials that meet both criteria, promoting better overall outcomes.

3. Empower Designers: LLMs can aid designers with limited material knowledge by offering data-driven recommendations. By understanding context and constraints, these models guide designers toward informed choices.

4. Early Intervention: Integrating LLMs early in the design cycle allows materials engineering experts to make informed decisions. By considering material properties, environmental impact, and cost factors, we aim to optimize material selection from the outset.

More specifically, this project is guided by the following research questions:

1. What patterns emerge in engineers' material selection tasks across various design contexts and criteria?

   Understanding these patterns is crucial for developing effective LLM-based systems that mimic human expertise.

2. Do LLM-based material selection systems accurately emulate the decision-making patterns exhibited by human engineers?

   Evaluating how well LLMs replicate human decision-making processes is essential for determining their efficacy and identifying areas for further development.

We address these research questions through two primary threads of work. First, we conduct a user survey involving domain experts in which we capture their preferences for different material types under varying design requirements and contexts. This data forms an empirical baseline against which to evaluate the performance of our LLM-based system and create a ground truth dataset for future research in this domain. In the second thread of work, we prototype an LLM pipeline for performing material selection and compare the LLM recommendations directly to the survey results from domain experts.

The remainder of this paper is organized as follows. In Section 2 we review work relevant to the major themes of this research. In Section 3 we introduce the overall methodology that we employ, detailing both the user survey and the LLM pipeline. Section 4 details the results from the survey and comparison, and Section 5 concludes the paper with a discussion of future work and limitations. The survey data and the LLM pipeline are available online[1].

2. BACKGROUND

In this section we review works related to material selection and its challenges, large language models and their application to design, and motivation to work on this problem.

2.1 Significance and Challenges in Material Selection

Material selection is a critical part of designing and producing any physical object. Material selection occurs in the early stages of the design workflow and maintains relevance beyond the useful life of a product. Materials directly influence the functionality, aesthetics, economic viability, manufacturing feasibility, and ultimately its environmental impact of a design [14–16]. M. F. Ashby is often cited for presenting a systematic approach to materials selection through the use of bubble plots, known as "Ashby" diagrams which allow a designer to evaluate up to two material properties to identify those materials that perform above a desired threshold [17]. This approach requires an intimate understanding of a product's design intent, the design priorities (such as low mass), constraints (manufacturing process), and other requirements relevant to the object being designed (industry regulations). In recent years, additional factors have become increasingly important to consider too. Sustainability, for example, is a growing global concern, and manufacturing alone is reported to contribute significantly to resource consumption and greenhouse gas emissions. Thus, selecting materials with lower environmental impact, such as recycled content or those requiring less energy to produce, aligns with ethical practices and growing consumer expectations [18–20]. Material availability is also becoming a critical consideration due to supply chain disruptions, geopolitical challenges, or regulations on material use. The growing complexity of design requirements, does not reduce the implications of improper material selection which can lead to increased overall costs, product failure, or greater environmental harm [21].

In product design, material selection can be broken down into a general five-step procedure: (1) establishing design requirements, (2) screening materials, (3) ranking materials, (4) researching material candidates, and (5) applying constraints to the selection process [22]. Performance indices and material property charts, called Ashby diagrams, are often used to visualize, filter, and cluster materials [22, 23].

Traditionally, material selection has relied heavily on engineering intuition and familiarity with existing materials. Particularly in industries with less prescriptive standards or specifications [24, 25]. Even with Ashby's systematic approach to material selection, the process is non-trivial and can still leave designers with uncertainty as to how well a candidate material will perform in reality [17, 23, 26]. Data and knowledge are essential, without which, limited exploration of alternative or innovative options

[1] https://github.com/cmudrc/LLM-for-Material-Selection

can occur leading to sub-optimal designs [27, 28] . While established methods like Ashby's can guide designers and encourage them to consider a wider range of possibilities, material databases [29] cannot often account for the ever-growing universe of materials and broadening design considerations outlined thus far. Selection can also be subjective, potentially overlooking promising new materials simply because designers are unfamiliar with them [30, 31] . Uncertainty regarding the performance of novel materials can further hinder their adoption. Additionally, manufacturing innovations like additive manufacturing are allowing previously unfeasible materials to now become viable options [32]. This highlights the need for a data-driven approach to material selection, one that can objectively evaluate a broader range of options while considering the complex interplay of design requirements and provide insights when selecting a particular option [33]. Large Language Models (LLMs) offer a powerful new tool for material selection. By learning from vast datasets of past design experiences and material properties, LLMs can provide valuable insights that would otherwise require extensive research or experimentation.

2.2 Automating Material Selection with Machine Learning and Large Language Models

The process of selecting materials for engineering applications has traditionally been a complex task that requires a deep understanding of both the materials and the specific application requirements, and has relied heavily on the expertise of engineers and materials scientists. Over the years, research has been done to automate this process, targeting the selection of materials for specific types of objects (e.g., nozzles, beams) and design functions (e.g., heat transfer and storage), often framing material selection as an optimization challenge [34–41].

While initial efforts to automate material selection have primarily utilized numerical methods and traditional optimization techniques, there has been a shift towards incorporating machine learning, particularly neural networks, into this process. These approaches, however, often fall short in ranking the suitability of selected materials, limiting their practical utility [42]. A notable exception is the work by Zhou *et al.*, which integrates a two-layer neural network with a genetic algorithm to select sustainable materials, demonstrating the approach through the design of a drink container [43]. Similarly, Chandrasekhar *et al.* employ a variational autoencoder in conjunction with a geometry encoder neural network, allowing for the simultaneous optimization of both the material and the geometry of a beam structure [38]. More recent work has leveraged large collections of CAD data with material labels and used graph neural networks to rank the most appropriate materials with a manufacturing- and class-agnostic method [44, 45].

Advancements in the natural language processing field around transformer-based architectures, coupled with training models on larger and larger datasets, have resulted in several pre-trained Large Language Models (LLMs) capable of mimicking human language, which appear to exhibit emergent reasoning capabilities [1–6]. In the design engineering domain, recent work has looked at leveraging LLMs to support designers during the conceptual design stage [7–9], as well as for detail design [10–13]. In regards to material selection, LLMs have been used to select appropriate materials from an Ashby chart [10], assist with selecting materials for building components [46], and propose appropriate manufacturing methods [47]. LLMs have also been fine-tuned on text extracted from a material textbook to aid in material-related design tasks [48].

In this work, we contribute to existing literature around material selection with LLMs by collecting a dataset with material rankings by experts for various design objects and criteria, and comparing them to a simple LLM baseline.

3. METHODOLOGY

In this section, we elaborate on the methodology that we used to answer our guiding research questions. In the first step 3.1, we gathered materials selection perspectives from professionals through an online survey - addressing the first research question. Following the responses, we designed a pipeline to query material selection preferences from a language model-based system 3.2 - addressing a part of the second research question. In the final stage 3.3, we compare both types of responses against each other, which allows us to fully answer the second research question.

3.1 Online Survey

To validate the outputs from an LLM-based system [49], we carried out an online survey among professionals in design, material science, engineering, and related fields. Specifically, our goal was to get responses from people with varied experiences in the field of material selection for mechanical design. We utilized Qualtrics to design our survey and survey was distributed through the Autodesk Research Community.

The survey consisted of 4 design cases (**Kitchen Utensil Grip**, **Spacecraft Component**, **Underwater Component**, and **Safety Helmet for Sport**) and 4 design criteria (**Lightweight**, **Heat Resistant**, **Corrosion Resistant** and **High Strength**) combined in a full factorial experimental design to produce 16 scenario-based questions. In each question, participants were asked to score a set of materials (**steel**, **aluminum**, **titanium**, **glass**, **wood**, **thermoplastic**, **elastomer**, **thermoset**, and **composite**) on a scale from 0 to 10, with 0 being unsatisfactory in the specific application and 10 being an excellent choice. These material categories were chosen to cover a breadth of design use cases, to find a balance between high-level and low-level material categories, and to limit the length of the survey. An example of a survey question is shown in Figure 1. The survey also collected basic demographic information to ensure that participants had the necessary knowledge and background to provide strong preferences for material selection.

The survey was distributed to professionals who have worked as materials scientists, materials engineers, design engineers, or related fields, via the Autodesk Research Community network. The survey remained accessible for 20 days.

3.2 Large Language Model Design

In this work, we used OpenAI's GPT-4 API to score all 9 material families across the same 16 design problems presented in the survey.

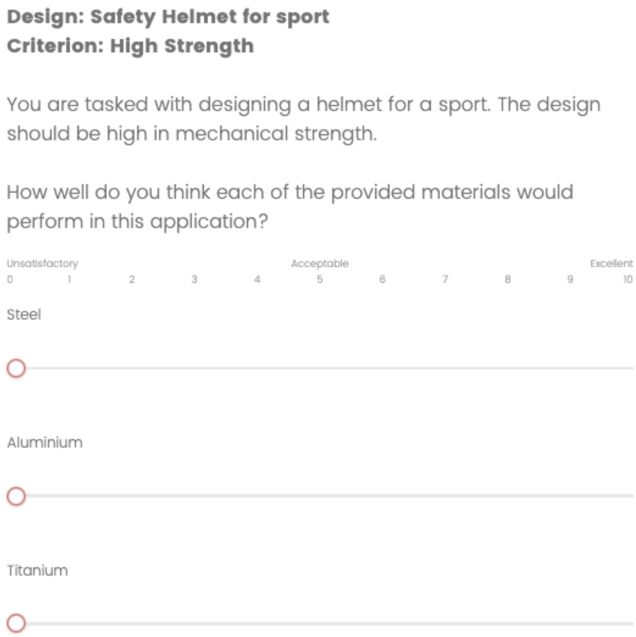

FIGURE 1: Example of a question asked on the survey, missing the remaining sliders allowing participants to select a value from 1-10. The 16 questions asked in the survey were created by taking all possible combinations of design cases and criteria. In all the questions, the only change made is the highlighted text, Design and Criterion.

We modified the questions from the survey to constrain the output to be in a standard JSON format to facilitate comparison with the numerical values from the survey responses. To do so, we employed the best practices described in the OpenAI API [50].

An example prompt is shown below, modified to add context on how the output should be presented.

> You are given a problem statement to assist a designer as below: The information below is provided to you delimited by triple backticks
>
> Design: ”’{design_choice}”’ Criterion: ”’{criterion}”’
>
> You are tasked with designing the grip of design_choice which should be criterion.
>
> How well do you think each of the provided materials would perform in this application?
>
> As a materials science and design engineer with experience in this field, you are supposed to give a score between 0-10 for each of the options provided below. This score should be how applicable each material family would be for this design case. 0 would be unacceptable and 10 would be excellent for this use case as mentioned in the question.
>
> Here are the material families to score on: ”’{material_families}”’
>
> The score is intended on a viability perspective, so the focus should be on how well the material satisfies the design and criterion pair.
>
> Output should be of a JSON format, use the following format: [...]

GPT-4 is capable of performing zero-shot learning [51], a technique used in NLP that allows a model to perform a task that it was not explicitly trained to do [52]. Given a task it has never seen before, it is often capable of producing a satisfactory output [53].

We deploy a zero-shot approach in all our pipeline tasks to get an output directly without providing any examples. The example prompt shown previously is also an example of a zero-shot prompt.

3.3 Evaluation

To evaluate the performance of the LLM in replicating the decision-making patterns exhibited by human experts, we conducted a comparative analysis between the LLM outputs and the survey responses. This analysis aimed to address our second research question: Do LLM-based material selection systems accurately emulate the decision-making patterns exhibited by human engineers?

First, we compiled the survey responses and the corresponding LLM outputs into a structured dataset, ensuring consistent formatting and alignment between the two data sources.

Next, we calculated the mean scores and standard deviations for each material family, segregated by the survey responses and the LLM outputs. These values were then plotted using error bar charts (Figure 2), allowing us to visually compare the central tendencies and variations between the two data sources.

To gain deeper insights into the distribution of scores, we performed a quartile analysis on both the survey data and the LLM outputs. Box-and-whisker plots (Figure 3) were generated to visualize the medians, interquartile ranges (IQRs), and outliers for each material family. This analysis enabled us to assess the skewness, variability, and the central tendency regions of the data, providing a more comprehensive understanding of the LLM's performance, and as a way to summarize the variable's distribution based on five values: minimum, first quartile, median, third quartile, and maximum [54].

Finally, building upon the quartile analysis, we evaluated the symmetry and skewness of the score distributions for each material family. Tables 1 and 2 summarize these characteristics for the survey data and the LLM outputs, respectively. This assessment helped us identify potential biases or deviations from the expected distributions.

By employing these evaluation techniques, we aimed to comprehensively assess the LLM's ability to replicate the decision-making patterns exhibited by human experts in material selection tasks. The comparative analysis between the LLM outputs and the survey data provided valuable insights into the strengths and limitations of the LLM-based system, informing future research directions and potential improvements.

4. RESULTS AND DISCUSSION

In this section, we answer our research questions and evaluate the proximity of the answers given by the language model to those provided by humans through the survey. Additionally, we explore how the outputs of the language model change in different aggregated contexts.

In total, 132 responses were received. Most of the respondents had previously worked in the field of material selection and were familiar with the material selection process. Approximately 90% of the participants were familiar with the material selection process. On average, respondents had 16 years of experience working as a materials scientist, materials engineer, design engineer, or a related designation.

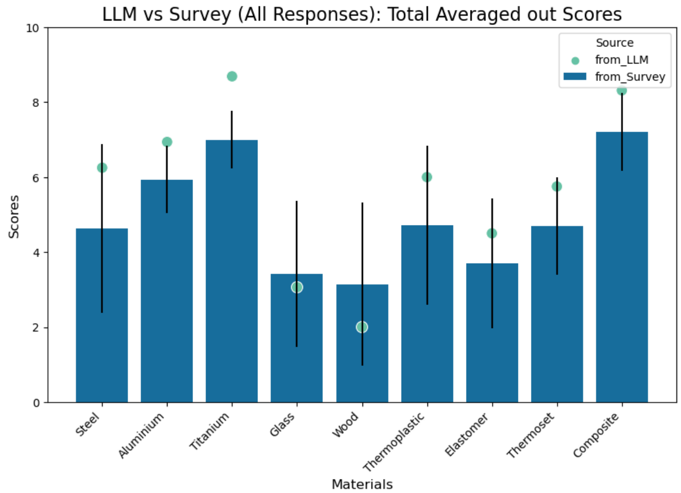

FIGURE 2: Comparison of averaged survey scores and large language model - All Design Cases and Criteria combined. Scores are compared for each material family. The results of the survey are shown in dark blue, and the results from the large language model are shown as a light blue dot. The error bars are the standard deviation of the survey results. We notice that apart from the material family Titanium, the output from the Large Language Model lies within the standard deviation of the outputs from the survey.

4.1 Total Aggregated Results

Figure 2 provides a comparison between the mean scores obtained from the survey across all questions and the mean scores of the output of the LLM, aggregated by material types. The Titanium and Composite materials are consistently scored higher by both survey respondents and the LLM. This can be attributed to the fact that cost was not a constraint in any of the questions asked. The consistent choice of composite for multiple design cases and criteria shows us the patterns engineers or professionals exhibit in the field of material selection.

As seen in Figure 2, the scores given the LLM lie within ± 1.0 standard deviation for all materials except for titanium. This shows that on average, the LLM can capture the patterns emerging from human thought processes and biases and emerge as a good companion. We also see that in most cases the LLM score is higher than the mean survey score; the exceptions to this trend are wood and glass. we notice that the LLM score is less than the survey score. This suggests that the LLM may be biased scores since historically the use of wood and glass has not been very high for the design cases used here. Although most of the scores from the LLM lie within the standard deviation, we also note substantial variance in survey responses in Figure 2. We attribute this large variance to the open-ended survey questions, which might not provide enough context about the design scenario for material experts to agree.

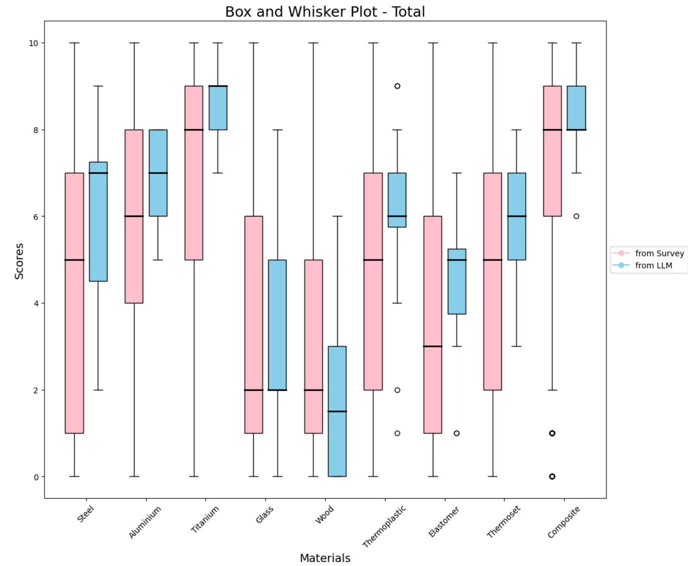

FIGURE 3: Quartile Comparison of survey scores and large language model - All Design Cases and Criteria combined. Scores are compared for each material family. The survey results are shown in pink box plots, and the results from the large language model are shown in blue box plots.

We performed a quartile analysis to examine the spread of the LLM scores away from the median value of the survey results. Figure 3 shows box-and-whisker plots, aggregated by material type. This plot shows the median, first, and third quartile using a colored rectangle. The whiskers extend from the box to the farthest data point that lies within 1.5x the interquartile range (IQR) from the box. The outlier points are those plotted beyond the whiskers. The scores from the language model are plotted in the same way. These plots allow us to better understand the skewness, variability, and interquartile range to verify if the LLM scores lie within the quartile ranges of the data computed from the survey.

Taking a closer look at figure 3, we compare the medians with the mean and assess the skewness material-wise. Table 1 shows symmetry and skewness information for the survey data, and Table 2 for the LLM data.

Material	Symmetry	Skewness
Steel	No	Negative
Aluminium	Yes	None
Titanium	No	Negative
Glass	No	Positive
Wood	No	Positive
Thermoplastic	No	Negative
Elastomer	No	Positive
Thermoset	No	Negative
Composite	No	Negative

TABLE 1: Table of symmetry and skewness for survey data

The skewness of different material families from the survey shows us the distribution of data. For example, steel has more variability in the lower scores than the higher scores. One take-

Material	Symmetry	Skewness
Steel	No	Negative
Aluminium	Yes	None
Titanium	No	Negative
Glass	No	Positive
Wood	Yes	None
Thermoplastic	No	Positive
Elastomer	No	Negative
Thermoset	Yes	None
Composite	No	Positive

TABLE 2: Table of symmetry and skewness for LLM data

away is that most of the IQRs for the LLM scores lie well within the IQRs of the survey data. This indicates that a score from the LLM is a high-probability choice since it lies in the central tendency region. This indicates that the Language Model even in its zero-shot form, can provide useful insights on material selection and emulates the patterns displayed by the expert survey respondents.

However, the median LLM scores do not match those of the survey results. This can be attributed to various factors outside of the scope of this work, from model hallucination to the model not being trained specifically on material data, to the inefficiency of the zero-shot inference method [55].

4.2 Limitations and Future Work

While our results are encouraging, it is important to acknowledge the limitations of this study. Our analysis focused on a specific set of design cases and criteria. To fully leverage the potential of LLMs in material selection, future work should expand the scope of the investigation to encompass both a broader and a more specific range of design scenarios and material families, to mitigate the large variance seen in survey responses. Also, more work should be done to evaluate other models, prompt engineering techniques, fine-tuning methods, and assess how parameters like temperature affect LLM accuracy. Lastly, more work should be done to quantitatively evaluate the performance of LLMs in this material selection task.

5. CONCLUSION

By integrating LLMs into the material selection process and evaluating their performance, this research provides insights and tools to enhance the efficiency and effectiveness of material selection in engineering design. Through a combination of expert evaluations and data-driven analysis, we seek to establish a framework for leveraging LLMs to support informed decision-making in material selection tasks.

Our findings demonstrate that, on average, the LLM outputs align closely with the mean scores obtained from the survey of professionals, lying within the standard deviation for eight out of nine material families. This alignment suggests that LLMs can effectively capture the inherent biases and thought processes involved in material selection, and could serve as valuable companions in the decision-making process.

Furthermore, our quartile analysis revealed that the interquartile range (IQR) of LLM scores often falls within the central tendency region of the survey data, indicating a high probability that the LLM's recommendations align with human experts' judgments. This consistency underscores the potential of LLMs to provide reliable and data-driven insights, facilitating more informed material selection decisions.

Overall, this research represents a significant step toward leveraging the capabilities of LLMs in material selection, paving the way for more efficient and effective decision-making in engineering design. By continuously refining and improving these models, we can empower designers with data-driven tools that facilitate informed material choices, ultimately leading to better product performance, cost optimization, and sustainability.

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